

FIG. 1A

	Atom	Туре	Resid	#	<u>x</u>	Ā	$\underline{\mathbf{z}}$	<u>0cc</u>	B
ATOM	1	CB	VAL	44	-1.554	11.775	58.841	1.00	44.68
ATOM	2	CG1		44	-0.373	12.518	59.504	1.00	41.59
ATOM	3		VAL	44	-2.770	12.693	58.662	1.00	38.80
ATOM	4	C	VAL	44`	-0.036	11.928	56.766	1.00	45.09
MOTA	5	0	VAL	44	0.936	11.355	56.264	1.00	41.95
MOTA	6	N	VAL	44	-0.692	9.711	57.661	1.00	46.59
ATOM	7	CA	VAL	44	-1.140	11.123	57.467	1.00	45.20
ATOM	8	N	ASP	45	-0.196	13.252	56.744	1.00	45.56
MOTA	9	CA	ASP	45	0.749	14.177	56.127	1.00	46.19
ATOM	10	CB	ASP	45	0.318	15.615	56.445	1.00	50.81
ATOM	11	CG	ASP	45	0.477	16.559	55.257	1.00	54.31
MOTA	12		ASP	45	1.579	16.604	54.657	1.00	54.34 53.14
MOTA	13		ASP	45	-0.504	17.269	54.936	1.00 1.00	45.23
MOTA	14	C	ASP	45	2.222	13.969	56.530 55.832	1.00	41.27
MOTA	15	0	ASP	45	3.125	14.433 13.286	57.654	1.00	44.70
MOTA	16	N	asn asn	46 46	2.459 3.816	13.200	58.127	1.00	40.32
ATOM	17 18	CA CB	ASN ASN	46	3.821	12.654	59.616	1.00	44.41
ATOM ATOM	· 19	ÇG	ASN	46	2.903	11.483	59.953	1.00	48.13
ATOM			ASN ·	46	2.249	10.903	59.080	1.00	51.07
MOTA	21		ASN	46	2.836	11.147	61.233	1.00	47.12
ATOM	.22	C	ASN	46	4.511	11.933	57.311	1.00	37.04
ATOM	23	ō	ASN	46	5.742	11.873	57.257	1.00	33.54
ATOM	24	N	GLN	47	3.715	11.069	56.690	1.00	31.75
ATOM	25	CA	GLN	47	4.253	10.008	55.855	1.00	32.28
ATOM	26	CB	GLN	47	3.180	8.964	55.586	1.00	32.94
ATOM	27	CG	GLN	47	2.635	8.292	56.827	1.00	35.16
MOTA	28	CD	GLN	47	1.600	7.245	56.492	1.00	37.29
MOTA	29	OE1		47	0.412	7.411	56.777	1.00	39.51
MOTA	30	NE2	GLN	47	2.042	6.161	55.861	1.00	38.10
MOTA	31	C	GLN	47	4.720	10.608	54.527	1.00	32.61
ATOM	32	0	GLN	47	5.560	10.031	53.823	1.00	34.45
MOTA	33	N	PHE	48	4.156	11.770	54.202	1.00	30.02 24.00
MOTA	34	CA	PHE	48	4.458	12.503	52.977	1.00 1.00	19.63
ATOM	35	CB	PHE	48	3.173	13.045 11.982	52.364 51.986	1.00	23.41
MOTA	36	CG	PHE	48	2.188	11.442	52.942	1.00	18.66
MOTA	37	CD1	PHE PHE	48	1.336 2.089	11.541	50.664	1.00	23.94
MOTA	38 39		PHE	48 48	0.391	10.471	52.596	1.00	20.60
MOTA MOTA	40	CE2		48	1.149	10.569	50.294	1.00	18.66
MOTA	41	CZ	PHE	48	0.292	10.032	51.266	1.00	23.76
ATOM	42	C	PHE	48	5.387	13.682	53.235	1.00	22.48
ATOM	43	ō	PHE	48	5.876	13.876	54.346	1.00	27.78
ATOM	44	N	TYR	49	5.659	14.434	52.173	1.00	19.53
MOTA	45	CA	TYR	49	6.493	15.620	52.225	1.00	15.88
ATOM	46	CB	TYR	49	7.939	15.255	52.551	1.00	11.81
MOTA	47	CG	TYR	49	8.848	14.994	51.384	1.00	16.74
MOTA	48	CD1	TYR	49	9.885	15.869	51.093	1.00	21.41
ATOM	49		TYR	49	10.800	15.595	50.073	1.00	22.47
ATOM	50		TYR	49	8.735	13.837	50.622	1.00	20.14
MOTA	51	CE2		49	9.653	13,555	49.594	1.00	20.86
MOTA	52	CZ	TYR	49	10.681	14.436	49.332	1.00	22.92
ATOM	53	OH	TYR	49	11.617	14.156	48.361	1.00	25.56
MOTA	54	C	TYR	49	6.376	16.346	50.892	1.00	20.03
MOTA	55	0	TYR	49	6.214	15.715 17.673	49.847 50.934	1.00	18.79
MOTA	56 57	N	SER	50	6.441	18.486	49.733	1.00	14.86
ATOM	57	CA	SER	50	6.301	70.400	22.133	4.00	74.00



#### FIG. 1B

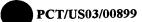
ATOM	58	СВ	SER	50		5.456	19.723	50.017	1.00	15.67
MOTA	59	OG	SER	50		4.087	19.385	50.146	1.00	17.38
ATOM	60	С	SER	50		7.577	18.909	49.048	1.00	18.39
ATOM	61	0	SER	50		8.606	19.149	49.685	1.00	18.03
MOTA	62	N	VAL	51		7.494	18.983	47.723	1.00	23.30
MOTA	63	CA	VAL	51		8.614	19.396	46.894	1.00	27.03
MOTA	64	CB	VAL	51		9.213	18.217	46.082	1.00	27.90
MOTA	65	CG1	VAL	51		10.674	18.504	45.755	1.00	30.77
ATOM	66	CG2	VAL	51		9.088	16.907	46.852	1.00	31.13
ATOM	67	С	VAL	51		8.104	20.459	45.931	1.00	27.87
ATOM	68	0	VAL	51		6.958	20.400	45.476	1.00	29.93
MOTA	69	N	GLU	52		8.930	21.468	45.672	1.00	29.63
ATOM	70	CA	GLU	52		8.543	22.538	44.757	1.00	27.26
MOTA	71	CB	GLU	52		9.072	23.897	45.221	1.00	29.95
ATOM	72	CG	GLU	52		8.638	25.037	44.300	1.00	36.89
ATOM	73	CD	GLU	52		9.302	26.360	44.619	1.00	39.00
ATOM	74	OE1	GLU	52		8.691	27.156	45.363	1.00	41.58
ATOM	75	OE2	GLU	52		10.421	26.602	44.112	1.00	35.61
ATOM	76	С	GLU	52		9.072	22.253	43.367	1.00	22.35
MOTA	77	0	GLU	52		10.276	22.284	43.135	1.00	25.69
MOTA	78	N	VAL	53		8.167	21.946	42.450	1.00	20.71
ATOM	79	CA	VAL	53		8.533	21.672	41.070	1.00	22.02
MOTA	80	CB	VAL	53		8.191	20.215	40.679	1.00	21.57
MOTA	81		VAL	53		8.531	19.970	39.223	1.00	24.78
MOTA	82	CG2	VAL	53	٠	8.968	19.238	41.558	1.00	24.81
MOTA	83	С	VAL	53		7.819	22.668	40.148	1.00	23.76
MOTA	84	0	VAL	53		6.686	22.434	39.700	1.00	24.98
MOTA	85	N	GLY	54		8.471	23.803	39.909	1.00	15.00
MOTA	86	CA	GLY	54		7.892	24.820	39.057	1.00	12.96
ATOM	87	C	GLY	54		6.635	25.424	39.651	1.00	12.55
MOTA	88	0	GLY	54		6.643	25.866	40.789	1.00	16.27
MOTA	89	N	ASP	55		5.557	25.462	38.870	1.00	18.77
MOTA	90	CA	ASP	55		4.285	26.024	39.335	1.00	19.62
MOTA	91	CB	ASP	55		3.300	26.271	38.176	1.00	23.42
MOTA	92	CG	ASP	55		3.773	27.322	37.175	1.00	28.63
MOTA	93	OD1	. ASP	55		4.643	28.158	37.505	1.00	29.48
MOTA	94	OD2	ASP	55		3.232	27.317	36.045	1.00	24.85 17.02
ATOM	95	C	ASP	55		3.607	25.044	40.261	1.00	
ATOM	96	0	ASP	55		2.596	25.368	40.876	1.00	18.70
ATOM	97	N	SER	56		4.128	23.823	40.288	1.00	19.63
ATOM	98	CA	SER	56		3.560		41.086	.1.00	20.49
MOTA	99	CB	SER	56		3.424	21.502	40.197	1.00	19.15
MOTA	100	OG	SER	56		2.680	21.805	39.034	1.00	21.54
MOTA	101	C	SER	56		4.283	22.372	42.380	1.00	14.16
ATOM	102	0	SER	56		5.471	22.639	42.565	1.00	10.18
MOTA	103	N	THR	57		3.533	21.754	43.281	1.00	11.32
ATOM	104	CA	THR	<sub>.</sub> 57	•	4.083	21.282	44.539	1.00	15.55
ATOM	105	CB	THR	57		3.360	21.910	45.778	1.00	15.32
MOTA	106	OG	LTHR	57		3.485	23.339	45.751	1.00	
ATOM	107	CG2	2 THR	57		3.965	21.395	47.065	1.00	8.74
ATOM	108	С	THR	57		3.860	19.770	44.550	1.00	11.87
MOTA	109	0	THR	57		2.720	19.307	44.476	1.00	8.37
ATOM	110	N	PHE	58		4.945		44.542	1.00	9.07
ATOM	111	CA	PHE	58		4.836		44.592	1.00	15.67
ATOM	112	CB	PHE	58		5.958		43.795	1.00	20.52
ATOM	113	CG		58		5.601			1.00	25.17
MOTA	114	CD:	1 PHE	58		5.240			1.00	29.63
MOTA	115		2 PHE	58		5.631			1.00	29.62
ATOM	116		1 PHE	58		4.914	17.411	40.160	1.00	31.71

# FIG. 1C

ATOM	117	CE2	PHE	58	5.309	15.058	40.510	1.00	24.12
ATOM	118	CZ	PHE	58	4.949	16.104	39.663	1.00	25.51
MOTA	119	C	PHE	58	4.851	17.031	46.029	1.00	15.98
ATOM	120	0	PHE	58	5.895	17.015	46.684	1.00	13.06
ATOM	121	N	THR	59	3.676	16.667	46.531	1.00	18.04
ATOM	122	CA	THR	59	3.524	16.115	47.878	1.00	16.76
MOTA	123	СВ	THR	59	2.194	16.572	48.489	1.00	22.41
MOTA	124	OG1	THR	59	2.113	18.003	48.419	1.00	26.00
ATOM	125	CG2	THR	59	2.080	16.134	49.939	1.00	24.02
ATOM	126	C	THR	59	3.584	14.575	47.792	1.00	12.75
	127	0		· 59	2.572	13.904	47.586	1.00	6.67
ATOM		M.	VAL	60	4.783	14.020	47.938	1.00	12.07
MOTA	128		VAL	60	4.975	12.572	47.821	1.00	16.39
ATOM	129	CA			5.977	12.234	46.675	1.00	9.02
ATOM	130	CB	VAL	60				1.00	11.33
ATOM	131		VAL	60	5.416	12.643	45.336	1.00	2.00
ATOM	132		VAL	60	7.307	12.913	46.914		20.62
MOTA	133	C	LAV	60	5.435	11.813	49.076	1.00	
MOTA	134	0	VAL	60	5.896	12.397	50.057	1.00	24.40
ATOM	135	N	LEU	61	5.317	10.491	49.015	1.00	18.08
ATOM	136	CA	LEU	61	5.736	9.632	50.111	1.00	14.84
MOTA	137	CB	LEU	61	5.429	8.166	49.790	1.00	12.15
ATOM	138	CG	LEU	61	3.962	7.752	49.646	1.00	10.77
ATOM	139	CD1	LEU	61	3.888	6.332	49.096	1.00	8.34
ATOM	140	CD2	LEU	61	3.265	7.851	50.981	1.00	5.08
ATOM	141	C	LEU	61	7.235	9.799	50.292	1.00	13.78
MOTA	142	ō	LEU	61	7.968	9.936	49.318	1.00	15.00
ATOM	143	N	LYS	62	7.683	9.750	51.541	1.00	13.56
ATOM	144	CA	LYS	62	9.088	9.903	51.888	1.00	11.45
	145	CB	LYS	62	9.232	9.898	53.408	1.00	18.13
ATOM			LYS	62	8.642	11.124	54.072	1.00	25.67
MOTA	146	CG		62	8.801	11.061	55.587	1.00	33.51
MOTA	147	CD	LYS			12.419	56.243	1.00	35.54
MOTA	148	CE	LYS	62	8.556	12.377	57.734	1.00	42.33
ATOM	149	NZ	LYS	62	8.729				7.12
ATOM	150	C	LYS	62	10.068	8.918	51.253	1.00	
MOTA	151	0	LYS	62	11.291	9.085	51.362	1.00	4.58
ATOM	152	N	ARG	63	9.540	7.882	50.610	1.00	11.02
ATOM	153	CA	ARG	63	10.382	6.884	49.942	1.00	10.76
MOTA	154	CB	ARG	63	9.583	5.598	49.667	1.00	9.20
ATOM	155	CG	ARG	63	8.343	5.763	48.797	1,00	10.52
MOTA	156	CD	ARG	63	7.573	4.449	48.599	1.00	13.21
ATOM	157	NE	ARG	63	8.381	3.390	47.986	1.00	9.08
ATOM	158	CZ	ARG	63	7.891	2.244	47.514	1.00	8.35
ATOM	159		ARG	63	6.594	1.982	47.569	1.00	4.31
ATOM	160		ARG	63	8.710	1.344	46.992	1.00	6.68
	161	C	ARG	63	10.943	7.453	48.637	1.00	8.74
ATOM	162	o	ARG	63	12.047	7.115	48.229	1.00	7.79
ATOM				64	10.193	8.367	48.034	1.00	9.03
ATOM	163	N	TYR		10.193	9.010	46.786	1.00	11.96
MOTA	164	CA	TYR	64			46.068	1.00	7.77
MOTA	165	CB	TYR	64	9.301	9.451	45.771	1.00	2.00
ATOM	166	CG	TYR	64	8.389	8.297	45.151	1.00	2.00
MOTA	167	CD1		64	8.878	7.155			
MOTA	168	CE1		64	8.058	6.074	44.883	1.00	2.11
MOTA	169	CD2		64	7.042	8.328	46.120	1.00	2.00
ATOM	170	CE2	TYR	64	6.212	7.246	45.852	1.00	2.00
ATOM	171	CZ	TYR	64	6.731	6.119	45.234	1.00	6.29
ATOM	172	OH	TYR	64	5.931	5.032	44.955	1.00	11.87
ATOM	173	С	TYR	64	11.455	10.202	47.081	1.00	15.27
MOTA	174	0	TYR	64	10.971	11.288	47.394	1.00	19.73
MOTA	175	N	GLN	65	12.759	10.004	46.980	1.00	17.91
		-		-					

FIG. 1D

ATOM	176	CA	GLN	65	13.704	11.070	47.285	1.00	19.85
MOTA	177	CB	GLN	65	14.856	10.480	48.109	1.00	16.92
MOTA	178	CG	GLN	65	14.366	9.720	49.332	1.00	21.05
ATOM '	179	CD	GLN	65	15.462	8.956	50.046	1.00	29.96
ATOM	180	OE1	GLN	65	16.641	9.021	49.674	1.00	32.66
ATOM	181	NE2	GLN	65	15.081	8.231	51.091	1.00	32.03
MOTA	182	С	GLN	65	14.251	11.886	46.104	1.00	21.54
ATOM	183	0	GLN	65	14.269	11.430	44.966	1.00	26.33
ATOM	184	N	ALA	66	14.658	13.119	46.402	1.00	23.53
ATOM	185	CA	ALA	66	15.252	14.051	45.435	1.00	21.77
MOTA	186	CB	ALA	66	16.727	13.720	45.233	1.00	19.86
MOTA	187	С	ALA	66	14.573	14.204	44.078	1.00	17.68
ATOM	188	0	ALA	66	15.211	13.988	43.057	1.00	16.11
ATOM	189	N	LEU	67	13.322	14.656	44.061	1.00	15.00
ATOM	190	CA	LEU	67	12.600	14.829	42.805	1.00	14.02
MOTA	191	CB	LEU	67	11.111	15.059	43.056	1.00	4.58
ATOM	192	CG	LEU	67	10.370	14.361	44.185	1.00	2.00
ATOM	193		LEU	67	8.880	14.471	43.920	1.00	2.00
ATOM	194		LEU	67	10.789	12.921	44.291	1.00	4.73
ATOM	195	C	LEU	67	13.105	15.981	41.917	1.00	21.98
MOTA	196	0	LEU	67	13.107	17.146	42.330	1.00	26.10
MOTA	197	N	ALA	68	13.520	15.652	40.697	1.00	23.28
MOTA	198	CA	ALA	68	13.972	16.653	39.736	1.00	20.49
ATOM	199	CB	ALA	68	15.337	16.268	39.178	1.00	14.57
MOTA	200	C	ALA	68	12.906	16.677	38.631	1.00	23.80
MOTA	201	0	ALA	68	12.214	15.689	38.416	1.00	21.05
ATOM	202	N	PRO	69 60	12.707	17.826	37.966	1.00 1.00	28.37 31.49
ATOM	203	CD	PRO	69 60	13.222	19.182	38.224	1.00	27.06
MOTA	204	CA	PRO	69 69	11.687	17.858 19.359	36.914 36.669	1.00	28.04
ATOM	205	CB	PRO	69	11.486		37.932	1.00	28.91
ATOM	206 207	CG C	PRO PRO	69	12.005 12.140	20.022 17.175	35.633	1.00	28.24
ATOM ATOM	207	0	PRO	69	13.341	17.043	35.364	1.00	23.40
MOTA	209	Ŋ	ILE	70	11.153	16.705	34.874	1.00	31.91
ATOM	210	CA	ILE	70	11.355	16.052	33.580	1.00	38.18
ATOM	211	CB	ILE	70	10.869	14.587	33.607	1.00	34.66
ATOM	212	CG2	ILE	70	10.114	14.234	32.338	1.00	36.72
ATOM	213	CG1	ILE	70	12.073	13.670	33.822	1.00	31.51
ATOM	214	CD1	ILE	70	11.704	12.237	34.017	1.00	29.61
ATOM	215	C	ILE	70	10.549	16.863	32.563	1.00	40.38
ATOM	216	ō	ILE	70	10.937	16.993	31.402	1.00	43.43
ATOM	217	N	GLY	71	9.405	17.371	33.027	1.00	44.94
MOTA	218	CA	GLY	71	8.537	18.208	32.223	1.00	47.46
ATOM	219	C	GLY	71	7.578	17.485	31.304	1.00	48.54
ATOM	220	O	GLY	71	7.887	16.401	30.815	1.00	47.51
ATOM	221	N	SER	72	6.400	18.091	31.127	1.00	51.97
ATOM	222	CA	SER	72	5.307	17.630	30.253	1.00	53.80
MOTA	223	CB	SER	72	5.136	16.113	30.276	1.00	52.09
MOTA	224	OG	SER	72	5.997	15.516	29.320	1.00	55.01
ATOM	225	C	SER	72	3.971	18.307	30.555	1.00	53.60
ATOM	226	0	SER	72	3.776	18.723	31.719	1.00	56.25
ATOM	227	CB	GLN	75	-2.575	15.033	30.778	1.00	26.20
MOTA	228	CG	GLN	75	-2.224	13.624	31.177	1.00	27.29
ATOM	229	CD	GLN	75	-3.442	12.728	31.172	1.00	31.62
ATOM	230	OE1	GLN	75	-3.558	11.818	30.342	1.00	36.78
ATOM	231	NE2	GLN	75	-4.381	13.001	32.083	1.00	31.34
MOTA	232	С	GLN	75	-1.319	16.062	32.660	1.00	27.21
ATOM	233	0	GLN	75	-2.275	16.251	33.425	1.00	31.31
ATOM	234	N	GLN	75	-0.228	15.740	30.395	1.00	24.95



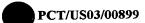
# FIG. 1E

ATOM	235	CA	GLN	75	-1.501	16.040	31.140	1.00	27.33
MOTA	236	N	GLY	76	-0.114	15.722	33.081	1.00	23.74
MOTA	237	CA	GLY	76	0.247	15.754	34.480	1.00	22.16
ATOM	238	C	GLY	76	1.684	16.234	34.382	1.00	26.62
MOTA	239	0	GLY	76	2.233	16.275	33.273	1.00	31.92
MOTA	240	N	ILE	77	2.294	16.662	35.482	1.00	20.67
MOTA	241	CA	ILE	77	3.679	17.096	35.390	1.00	16.35
ATOM	242	CB	ILE	77	4.019	18.301	36.308	1.00	19.61
MOTA	243	CG2	ILE	77	5.504	18.705	36.124	1.00	12.60
MOTA	244	CG1	ILE	77	3.160	19.521	35.953	1.00	17.46
MOTA	245	CD1	ILE	77	1.659	19.354	36.135	1.00	18.13
MOTA	246	C	ILE	77	4.453	15.843	35.762	1.00	14.34
ATOM	247	0	ILE	77	3.934	14.986	36.477	1.00	15.37
ATOM	248	N	VAL	78	5.645	15.678	35.203	1.00	13.70
ATOM	249	CA	VAL	78	6.446	14.487	35.472	1.00	13.92
MOTA	250	CB	VAL	78	6.613	13.639	34.176	1.00	13.49
ATOM	251	CG1	JAV	78	7.578	12.482	34.393	1.00	11.19
ATOM	252	CG2	VAL	78	5.249	13.122	33.730	1.00	6.97
ATOM	253	C	VAL	78	7.804	14.768	36.098	1.00	15.53
MOTA	254	0	VAL	78	8.587	15.567	35.577	1.00	16.48
ATOM	255	N	CYS	79	8.097	14.038	37.176	1.00	16.79
ATOM	256	CA	CYS	79	9.345	14.181	37.923	1.00	12.30
ATOM	257	CB	CYS	79	9.063	14.590	39.375	1.00	17.48
ATOM	258	SG	CYS	79	8.724	16.334	39.667	1.00	17.95
ATOM	259	С	CYS	79	10.189	12.915	37.951	1.00	7.69
ATOM	260	0	CYS	79	9.677	11.804	37.991	1.00	10.14
ATOM	261	N	ALA	80	11.496	13.113	37.907	1.00	4.10
ATOM	262	CA	ALA	80	12.462	12.040	37.970	1.00	13.15
MOTA	263	СВ	ALA	80	13.731	12.446	37.236	1.00	12.16
MOTA	264	C	ALA	80	12.772	11.840	39.452	1.00	21.14
ATOM	265	0	ALA	80	13.532	12.617	40.038	1.00	26.46
ATOM	266	N	ALA	81	12.211	10.798	40.055	1.00	21.98
ATOM	267	CA	ALA	81	12.458	10.536	41.472	1.00	21.56
MOTA	268	CB	ALA	81	11.139	10.221	42.180	1.00	17.84
ATOM	269	C	ALA	81	13.462	9.411	41.703	1.00	19.64
ATOM	270	ō	ALA	81	14.131	8.960	40.770	1.00	21.54
ATOM	271	N	TYR	82	13.609	9.029	42.972	1.00	20.19
ATOM	272	CA	TYR	82	14.474	7.929	43.381	1.00	20.94
MOTA	273	СВ	TYR	82	15.831	8.409	43.892	1.00	21.43
ATOM	274	CG	TYR	82	16.599	7.311	44.604	1.00	25.93
ATOM	275	CD1		82	17.105	6.218	43.907	1.00	29.90
ATOM	276		TYR	82	17.756	5.178	44.573	1.00	30.94
ATOM	277	CD2		82	16.772	7.337	45.985	1.00	25.81
ATOM	278	CE2	TYR	82	17.420	6.303	46.653	1.00	23.76
ATOM	279	cz	TYR	82	17.903	5.230	45.946	1.00	30.58
ATOM	280	ОН	TYR	82	18.500	4.196	46.618	1.00	29.44
ATOM	281	C	TYR	82	13.758	7.163	44.480	1.00	20.67
MOTA	282	Ö	TYR	82	13.568	7.684	45.576	1.00	23.05
ATOM	283	N	ASP	83	13.371	5.927	44.183	1.00	17.38
ATOM	284	CA	ASP	83	12.667	5.098	45.145	1.00	15.03
ATOM	285	CB	ASP	83	11.861	4.034	44.434	1.00	14.45
MOTA	286	CG	ASP	83	10.693	3.567	45.247	1.00	17.56
ATOM	287		ASP	83	10.777	3.604	46.496	1.00	18.87
ATOM	288	OD2		83	9.681	3.177	44.632	1.00	22.51
ATOM	289	C	ASP	83	13.648	4.432	46.088	1.00	19.10
ATOM	290	0	ASP	83	14.315	3.470	45.710	1.00	19.53
MOTA	291	И	ALA	84	13.667	4.905	47.335	1.00	18.37
ATOM	292	CA	ALA	84	14.569	4.401	48.367	1.00	13.42
ATOM	293	CB	ALA	84 84	14.492	5.290	49.595	1.00	16.90
111 OL1	233	C15	TH	04	エマ・セフム	3.230	20.000	00	10.50



## FIG. 1F

ATOM	294	С	ALA	84	14 264	2 067	40 727		
ATOM	295		ALA	84	14.264 15.178	2.967 2.180	48.737	1.00	7.60
ATOM	296		VAL	85	12.983		48.967	1.00	7.42
ATOM	297		VAL	85		2.622	48.754	1.00	2.00
ATOM	298		VAL		12.557	1.270	49.086	1.00	11.88
ATOM	299		VAL L VAL	85	11.023	1.208	49.289	1.00	15.00
				85	10.608	-0.176	49.738	1.00	18.62
ATOM	300		Z VAL	85	10.588	2.250	50.314	1.00	11.37
ATOM	301	C	VAL	85	12.979	0.217	48.042	1.00	15.24
ATOM	302	0	VAL	85	13.496	-0.845	48.391	1.00	17.38
ATOM	303	N	LEU	86	12.772	0.533	46.765	1.00	17.84
MOTA	304	CA	LEU	86	13.118	-0.369	45.664	1.00	13.79
MOTA	305	CB	LEU	86	12.144	-0.177	44.515	1.00	12.13
MOTA	306	CG	LEU	86	10.866	-1.006	44.534	1.00	12.71
MOTA	307		. LEU	86	10.245	-1.065	45.909	1.00	16.53
MOTA	308		LEU	86	9.910	-0.409	43.536	1.00	14.81
MOTA	309	C	LEU	86	14.529	-0.191	45.129	1.00	17.04
MOTA	310	0	LEU	86	15.020	-1.035	44.382	1.00	21.60
MOTA	311	N	ASP	87	15.186	0.891	45.530	1.00	18.90
MOTA	312	CA	ASP	87	16.539	1.204	45.079	1.00	23.81
MOTA	313	CB	ASP	87	17.543	0.151	45.551	1.00	22.37
ATOM	314	CG	ASP	87	18.984	0.609	45.381	1.00	30.15
MOTA	315	OD1	ASP	87	19.271	1.797	45.637	1.00	29.63
ATOM	316		ASP	87	19.836	-0.212	44.981	1.00	35.59
MOTA	317	C	ASP	87	16.664	1.391	43.567	1.00	25.14
ATOM	318	0	ASP	87	17.634	0.937	42.948	1.00	28.93
ATOM	319	N	ARG	88	15.691	2.071	42.979	1.00	24.77
ATOM	320	CA	ARG	88	15.710	2.335	41.546	1.00	23.82
ATOM	321	СВ	ARG	88	14.940	1.270		1.00	
ATOM	322	CG	ARG	88	13.481	1.152	41.185	1.00	21.43
ATOM	323		ARG	88	12.588	0.723			26.04
ATOM	324	NE.	ARG	88	13.157		40.042	1.00	35.46
ATOM	325	CZ	ARG	88	12.473	-0.353	39.224	1.00	43.22
ATOM	326		ARG	88	11.185	-1.048	38.314	1.00	43.53
ATOM	327		ARG	88		-0.796	38.104	1.00	42.29
ATOM	328	C	ARG	88	13.083	-1.977	37.583	1.00	47.38
ATOM	329	0	ARG		15.078	3.691	41.299	1.00	21.16
ATOM	330			88	14.143	4.080	41.995	1.00	19.00
ATOM	331	N	ASN	89	15.592	4.402	40.297	1.00	18.57
ATOM		CA	ASN	89	15.073	5.716	39.951	1.00	10.01
	332	CB	ASN	89	15.949	6.402	38.905	1.00	12.28
ATOM	333	CG	ASN	89	17.437	6.099	39.063	1.00	20.41
MOTA	334		ASN	89	17.838	4.942	39.186	1.00	31.61
ATOM	335		ASN	89	18.262	7.139	39.020	1.00	19.05
MOTA	336	C	ASN	89	13.716	5.447	39.344	1.00	4.86
ATOM	337	0	ASN	89	13.534	4.452	38.650	1.00	7.53
ATOM	338	N	VAL	90	12.740	6.277	39.675	1.00	5.33
ATOM	339	CA	VAL	90	11.399	6.127	39.128	1.00	2.00
ATOM	340	CB	VAL	90	10.408	5.600	40.186	1.00	4.37
ATOM	341		VAL	90	10.862	4.240	40.702	1.00	7.02
MOTA	34,2		VAL	90	10.254	6.597	41.321	1.00	6.06
ATOM	343	C	VAL	90	10.893	7.454	38.545	1.00	4.05
ATOM	344	0	VAL	90	11.662	8.397	38.347	1.00	5.5 <b>7</b>
MOTA	345	N	ALA	91	9.609	7.500	38.212	1.00	2.00
MOTA	346	CA	ALA	91	8.984	8.704	37.679	1.00	3.61
MOTA	347	CB	ALA	91	8.920	8.670	36.151	1.00	5.67
MOTA	348	С	ALA	91	7.589	8.771	38.270	1.00	10.32
ATOM	349	0	ALA	91	6.900	7.751	38.412	1.00	13.32
ATOM	350	N	ILE	92	7.193	9.976	38.657	1.00	12.22
ATOM	351	CA	ILE	92	5.889	10.198	39.257	1.00	13.29
MOTA	352	CB	ILE	92	6.063	10.804	40.697	1.00	15.08



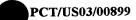
# FIG. 1G

ATOM	353	CG2	ILE	92	4.800	10.584	41.536	1.00	9.12
MOTA	354	CG1	ILE	92	7.269	10.161	41.400	1.00	14.98
ATOM	355	CD1	ILE	92	7.639	10.804	42.711	1.00	17.01
ATOM	356	C	ILE	92	5.133	11.181	38.368	1.00	12.70
ATOM	357	0	ILE	92	5.749	12.012	37.702	1.00	13.94
ATOM	358	N	LYS	93	3.811	11.055	38.323	1.00	10.80
MOTA	359	CA	LYS	93	2.993	11.962	37.534	1.00	12.68
ATOM	360	CB	LYS	93	2.523	11.301	36.238	1.00	18.72
ATOM	361	CG	LYS	93	1.678	12.217	35.356	1.00	26.15
ATOM	362	CD	LYS	93	1.476	11.675	33.953	1.00	33.36
ATOM	363	CE	LYS	93	0.568	10.453	33.920	1.00	38.49
ATOM	364	NZ	LYS	93	0.554	9.814	32.569	1.00	45.17
ATOM	365	C	LYS	93	1.800	12.403	38.364	1.00	12.16
ATOM	366	ō	LYS	93	1.090	11.582	38.936	1.00	12.27
	367	N	LYS	94	1.566	13.705	38.415	1.00	12.37
ATOM			LYS	94	0.467	14.226	39.214	1.00	13.50
MOTA	368	CA	LYS	94	0.933	15.404	40.080	1.00	11.86
ATOM	369	CB				15.759	41.148	1.00	14.06
ATOM ·	370	CG	LYS	94	-0.094	17.250	41.372	1.00	12.12
ATOM	371	CD	LYS	94	-0.275			1.00	15.03
MOTA	372	CE	LYS	94	0.889	17.881	42.073		21.64
ATOM	373	NZ	LYS	94	0.418	19.124	42.737	1.00	
ATOM	374	C	LYS	94	-0.760	14.657	38.442	1.00	13.08
ATOM	375	0	LYS	94	-0.704	15.562	37.616	1.00	18.01
ATOM	376	N	LEU	95	-1.877	14.017	38.741	1.00	14.19
MOTA	377	CA	LEU	95	-3.142	14.351	38.120	1.00	13.05
ATOM	378	CB	PEA	95	-3.913	13.090	37.718	1.00	17.09
ATOM	379	CG	LEU	95	-3.643	12.386	36.391	1.00	15.05
ATOM	380		LEU	95	-2.201	11.920	36.310	1.00	15.02
MOTA	381		LEU	95	-4.602	11.207	36.267	1.00	17.68
MOTA	382	C	LEU	95	-3.969	15.093	39.153	1.00	17.18
ATOM	383	0	LEU	95	-4.535	14.480	40.049	1.00	18.32
ATOM	384	N	SER	96	-4.030	16.412	39.035	1.00	17.90
ATOM	385	CA	SER	96	-4.814	17.212	39.958	1.00	16.67
MOTA	386	CB	SER	96	-4.283	18.645	40.036	1.00	20.30
ATOM	387	OG	SER	96	-2.903	18.681	40.351	1.00	30.22
ATOM	388	С	SER	96	-6.268	17.242	39.518	1.00	16.31
MOTA	389	0	SER	96	-6.567	17.551	38.369	1.00	23.36
MOTA	390	N	ARG	97	-7.164	16.915	40.443	1.00	13.24
ATOM	391	CA	ARG	97	-8.607	16.924	40.198	1.00	14.86
ATOM	392	CB	ARG	97	-9.164	18.349	40.326	1.00	17.53
ATOM	393	CG	ARG	97	-8.944	18.996	41.669	1.00	17.18
ATOM	394	CD	ARG	97	-9.733	20.285	41.788	1.00	19.58
MOTA	395	NE	ARG	97	-9.465	20.914	43.072	1.00	27.92
MOTĄ	396	CZ	ARG	97	-10.120	20.649	44.200	1.00	29.09
MOTA	397		ARG	97	-11.119	19.771	44.229	1.00	33.26
ATOM	398		ARG	97	-9.723	21.217	45.326	1.00	25.41
ATOM	399	C	ARG	97	-9.061	16.331	38.865	1.00	16.76
MOTA	400	0	ARG	97	-9.819	16.954	38.127	1.00	17.95
ATOM	401	N	PRO	98	-8.634	15.097	38.562	1.00	17.80
ATOM	402	CD	PRO	98	-7.815	14.196	39.385	1.00	18.27
ATOM	403	CA	PRO	98	-9.015	14.448	37.305	1.00	14.40
MOTA	404	CB	PRO	98	-8.280	13.110	37.378	1.00	14.74
ATOM	405	CG	PRO	98	-8.172	12.843	38.838	1.00	15.84
ATOM	405	C	PRO	.98	-10.523	14.275	37.128	1.00	14.36
ATOM	407	0	PRO	.98	-11.018	14.251	36.001	1.00	18.45
ATOM	408	N	PHE	96 99	-11.247	14.178	38.237	1.00	11.59
ATOM	409	CA	PHE	99	-12.702	14.005	38.240	1.00	8.51
ATOM	410	CB	PHE	99	-13.166	13.512	39.625	1.00	10.76
ATOM	411	CG	PHE	99 99 .	-12.577	14.301	40.775	1.00	11.82
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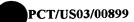
## FIG. 1H

MOTA	412	CD1	PHE	99	-11.334	13.954	41.297	1.00	9.19
MOTA	413	CD2		99	-13.211	15.456	41.248	1.00	11.64
MOTA	414	CE1	PHE	99	-10.718	14.753	42.255	1.00	10.55 3.04
MOTA	415	CE2	PHE	99	-12.604	16.266	42.210	1.00	3.04
MOTA	416	CZ	PHE	99	-11.354	15.918	42.711	1.00	
MOTA	417	С	PHE	99	-13.479	15.272	37.864	1.00	9.70 4.45
ATOM	418	0	PHE	99	-14.710	15.223	37.780	1.00	14.64
MOTA	419	N	GLN	100	-12.785	16.395	37.643	1.00	21.27
MOTA	420	CA	GLN	100	-13.453	17.660	37.286	1.00	21.59
MOTA	421	CB	GLN	100	-12.672	18.874	37.810	1.00	25.09
MOTA	422	CG	GLN	100	-12.635	18.961	39.332		29.38
MOTA	423	CD	GLN	100	-13.299	20.216	39.918	1.00	26.88
ATOM	424	OE1	GLN	100	-12.865	20.716	40.963	1.00	28.47
MOTA	425	NE2	GLN	100	-14.380	20.695	39.285	1.00	23.90
MOTA	426	C.	GLN	100	-13.798	17.854	35.808	1.00	24.03
MOTA	427	0	GLN	100	-14.617	18.721	35.468	1.00	25.19
MOTA	428	N	ASN	101	-13.181	17.054	34.942	1.00	24.30
ATOM	429	CA	ASN	101	-13.430	17.105	33.502	1.00	28.04
ATOM	430	CB	ASN	101	-12.143	17.447	32.743	1.00	
MOTA	431	CG	ASN	101	-12.352	17.515	31.241	1,00	31.27
MOTA	432	OD1	ASN	101	-12.109	16.543	30.531	1.00	37.00
MOTA	433	ND2	ASN	101	-12.801	18.666	30.751	1.00	32.53
MOTA	434	C	ASN	101	-13.933	15.738	33.069	1.00	21.66
MOTA	435	0	ASN	101	-13.186	14.767	33.103	1.00	20.60
ATOM	436	N	GLN	102	-15.191	15.676	32.643	1.00	19.05
ATOM	437	CA	GLN	102	-15.824	14.430	32.210	1.00	24.39
ATOM	438	CB	GLN	102	-17.060	14.741	31.372	1.00	27.49
MOTA	439	CG	GLN	102	-17.874	13.518	31.001	1.00	36.15
ATOM	440	CD	GLN	102	-18.898	13.166	32.066	1.00	42.89
MOTA	441	OE1	GLN	102	-19.578	14.048	32.600	1.00	43.41
MOTA	442	NE2	GLN	102	-19.022	11.874	32.375	1.00	41.93
MOTA	443	С	GLN	102	-14.929	13.474	31.413	1.00	23.63
MOTA	444	0	GLN	102	-15.050	12.257	31.548	1.00	24.99
ATOM	445	N	THR	103	-14.066	14.029	30.562	1.00	20.69
MOTA	446	CA	THR	103	-13.158	13.246	29.730	1.00	17.84
ATOM	447	CB	THR	103	-12.702	14.052	28.504	1.00	17.02
ATOM	448	OG1	THR	103	-13.839	14.415	27.718	1.00	19.48
ATOM	449	CG2	THR	103	-11.724	13.253	27.665	1.00	11.85
MOTA	450	C	THR	103	-11.905	12.815	30.480	1.00	20.98
ATOM	451	0	THR	103	-11.425	11.691	30.306	1.00	24.66
MOTA	452	N	HIS	104	-11.328	13.744	31.242	1.00	20.55
MOTA	453	CA	HIS	104	-10.129	13.466	32.035	1.00	15.76
MOTA	454	CB	HIS	104	-9.617	14.751	32.678	1.00	15.65
MOTA	455	CG	HIS	104	-8.759	15.578	31.780	1.00	10.94
MOTA	456	CD2	2 HIS	104	-7.423	15.789	31.776	1.00	18.06
MOTA	457	NDI	LHIS	104	-9.269	16.318	30.736	1.00	11.77
ATOM	458	CEI	LHIS	104	-8.283	16.953	30.127	1.00	19.65
MOTA	459	NE	2 HIS	104	-7.151	16.650	30.738	1.00	19.90
MOTA	460	C	HIS	104	-10.464	12.452	33.127	1.00	14.82
MOTA	461	0	HIS	104	-9.615	11.667	33.546		13.77
MOTA	462	N	ALA	105	-11.728	12.469	33.536		11.82
MOTA	463	CA	ALA	105	-12.252	11.602	34.565		8.37
ATOM	464	CB	ALA		-13.651	12.031	34.911		6.82
MOTA	465		ALA		-12.262	10.182	34.049		
MOTA	466		ALA	105	-11.449	9.353	34.459		
ATOM	467	N	LYS	, 106	-13.141				
MOTA	468	CA		•	-13.322				
ATOM	469	CB	LYS	106	-14.186				
MOTA	470	CG	LYS	106	-14.983	7.587	30.792	1.00	32.05



#### FIG. 1I

MOTA	471	CD	LYS	106	-15.989	7.883	29.669	1.00	38.01
MOTA	472	CE	LYS	106	-17.129	8.834	30.090	1.00	38.61
ATOM	473	NZ	LYS	106	-16.846	10.302	29.933	1.00	32.07 7.28
MOTA	474	C	LYS	106	-11.959	8.082	32.080	1.00	8.85
MOTA	475	0	LYS	106	-11.645	6.933	32.376	1.00	7.12
MOTA	476	N	ARG	107	-11.117	8.938	31.521	1.00	7.12
MOTA	477	CA	ARG	107	-9.782	8.547	31.126		
MOTA	478	CB	ARG	107	-9.051	9.740	30.503	1.00	6.80 12.16
MOTA	479	CG	ARG	107	-7.647	9.444	30.016	1.00	19.65
MOTA	480	CD	ARG	107	-7.115	10.583	29.136		28.47
MOTA	481	NE	ARG	107	-5.842	10.259	28.479	1.00 1.00	23.50
MOTA	482	CZ	ARG	107	-5.717	9.538	27.365	1.00	23.94
MOTA	483	-	ARG	107	-6.790	9.047	26.753		24.62
MOTA	484		ARG	107	-4.513	9.320	26.852	1.00	6.34
MOTA	485	C	ARG	107	-9.002	7.984	32.300	1.00	12.54
ATOM	486	0	ARG	107	-8.558	6.850	32.232	1.00	13.11
MOTA	487	N	ALA	108	-8.905	8.745	33.393	1.00	12.23
MOTA	488	CA	ALA	108	-8.160	8.341	34.600	1.00	16.56
MOTA	489	CB	ALA	108	-8.183	9.452	35.612	1.00 1.00	9.84
MOTA	490	С	ALA	108	-8.605	7.040	35.266		9.07
MOTA	491	0	ALA	108	-7.775	6.231	35.687	1.00 1.00	7.50
MOTA	492	N	TYR	109	-9.911	6.854	35.394	1.00	13.33
MOTA	493	CA	TYR	109	-10.441	5.651	36.001	1.00	19.72
MOTA	494	CB	TYR	109	-11.959	5.744	36.083	1.00	22.28
MOTA	495	CG	TYR	109	-12.603	4.518	36.669 37.908	1.00	23.99
MOTA	496		TYR	109	-12.213	4.035	37.906	1.00	25.88
MOTA	497	CE1		109	-12.825	2.929	36.001	1.00	22.06
MOTA	498	CD2		109	-13.623	3.862	36.554	1.00	21.88
MOTA	499	CE2		109	-14.241	2.752	37.785	1.00	26.78
MOTA	500	CZ	TYR	109	-13.838	2.292	38.341	1.00	33.91
MOTA	501	OH	TYR	109	-14.460	1.200	35.157	1.00	17.09
ATOM	502	С	TYR	109	-10.064	4.446 3.485	35.642	1.00	18.57
ATOM	503	0	TYR	109	-9.470	4.550	33.874	1.00	19.91
ATOM	504	N	ARG	110	-10.389	3.533	32.865	1.00	17.79
MOTA	505	CA	ARG	110	-10.157	4.125	31.511	1.00	29.51
MOTA	506	CB	ARG	110	-10.568	3.137	30.369	1.00	32.16
MOTA	507	CG	ARG	110	-10.758	3.137	29.095	1.00	29.67
MOTA	508	CD	ARG	110	-11.271	3.039	27.916	1.00	30.13
MOTA	509	NE	ARG	110	-10.935	3.039	27.350	1.00	29.42
MOTA	510	CZ	ARG	110	-9.733	3.786	27.843	1.00	31.13
ATOM	511		LARG	110	-8.756	2.204	26.342	1.00	29.18
MOTA	512	NH2		110	-9.482	3.044	32.823	1.00	16.76
MOTA	513	С	ARG	110	-8.714	1.842	32.828	1.00	16.62
MOTA	514	0	ARG	110	-8.458	3.973	32.798	1.00	15.33
MOTA	515	N	GLU	111	-7.766	3.616	32.735	1.00	17.28
ATOM	516	CA	GLU	111	-6.353		32.733	1.00	21.45
MOTA	517	CB	GLU	111	-5.498	4.878 5.932	31.598	1.00	20.21
MOTA	518	CG	GLU	111	-6.046	5.641	30.133	1.00	19.30
MOTA	519	CD	GLU	111	-5.777	5.984	29.672		8.75
MOTA	520		1 GLU	111	-4.670	5.124			22.37
MOTA	521		2 GLU	111	-6.683	2.853	33.977		16.99
MOTA	522	C	GLU	111	-5.913	2.000	_		
MOTA	523		GLU	111	-5.020				
MOTA	524		LEU	112	-6.538				
MOTA	525			112	-6.264				
MOTA	526			112	-6.919				
MOTA	527			112	-6.096				
MOTA	528	•	1 LEU	112	-4.658				
MOTA	529	CD	2 LEU	112	-6.815	5.140	39.307	1.00	74.10



#### FIG. 1J

ATOM	530	С	<b>LEU</b>	112	-6.819	1.151	36.435	1.00	12.99
MOTA	531	0	LEU	112	-6.126	0.199	36.801	1.00	6.73
MOTA	532	N	VAL	113	-8.048	1.006	35.965	1.00	6.24
MOTA	533	CA	VAL	113	-8.707	-0.275	35.893	1.00	6.98
MOTA	534	CB	VAL	113	-10.187	-0.076	35.500	1.00	7.10
ATOM	535	CG1	VAL	113	-10.870	-1.409	35.272	1.00	12.66
MOTA	536	CG2	VAL	113	-10.910	0.713	36.577	1.00	12.28
ATOM	537	C	VAL	113	-8.033	-1.212	34.874	1.00	11.22
ATOM	538	0	VAL	113	-7.904	-2.414	35.114	1.00	15.98
MOTA	539	N	LEU	114	-7.554	-0.646	33.770	1.00	14.36
ATOM	540	CA	LEU	114	-6.927	-1.423	32.707	1.00	16.13
MOTA	541	CB	LEU	114	-7.010	-0.679	31.375	1.00	15.67
MOTA	542	CG	LEU	114	-8.393	-0.629	30.753	1.00	12.06
ATOM	543	CD1	LEU	114	-8.282	0.021	29.404	1.00	17.14
MOTA	544	CD2	LEU	114	-8.937	-2.036	30.614	1.00	17.36
ATOM	545	С	LEU	114	-5.500	-1.846	32.931	1.00	16.07
ATOM	546	0	LEU	114	-4.999	-2.719	32.225	1.00	21.08
ATOM	547	N	MET	115	-4.836	-1.252	33.905	1.00	16.41
MOTA	548	CA	MET	115	-3.455	-1.617	34.149	1.00	16.95
ATOM	549	CB	MET	115	-2.727	-0.509	34.895	1.00	20.21
MOTA	550	CG	MET	115	-1.350	-0.250	34.333	1.00	19.72
MOTA	551	SD	MET	115	-0.698	1.312	34.874	1.00	28.78
ATOM	552	CE	MET	115	-1.885	2.433	34.130	1.00	25.09
MOTA	553	С	MET	115	-3.335	-2.950	34.871	1.00	16.08
MOTA	554	0	MET	115	-2.244	-3.499	34.991	1.00	18.48
ATOM	555	N	LYS	116	-4.472	-3.459	35.334	1.00	18.87
ATOM	556	CA	LYS	116	-4.542	-4.744	36.015	1.00	23.57
ATOM	557	CB	LYS	116	-5.706	-4.749	37.021	1.00	26.91
ATOM	558	CG	LYS	116	-5.551	-3.731	38.161	1.00	33.65
ATOM	559	CD	LYS	116	-6.631	-3.843	39.247	1.00	35.36
ATOM	560	CE	LYS	116	-7.921	-3.092	38.909	1.00	36.42
ATOM	561	NZ	LYS	116	-8.741	-3.743	37.845	1.00	37.10
ATOM	562	C	LYS	116	-4.767	-5.825	34.956	1.00	25.45
MOTA	563	0	LYS	116	-4.443	-6.995	35.162	1.00	24.99
ATOM	564	N	CYS	117	-5.306	-5.397	33.813	1.00	22.92
ATOM	565	CA	CYS	117	-5.613	-6.267	32.689	1.00	15.45
ATOM	566	CB	CYS	117	-6.767	-5.679	31.890	1.00	12.92
MOTA	567	SG	CYS	117	-8.238	-5.322	32.853	1.00	21.59
MOTA	568	C	CYS	117	-4.451	-6.493	31.732	1.00	15.36
ATOM	569	0	CYS	117	-4.565	-7.300	30.814	1.00	20.75
ATOM	570	N	VAL	118	-3.344	-5.784	31.929	1.00	17.19
ATOM	571	CA	VAL	118	-2.185	-5.916	31.041	1.00	19.32
MOTA	572	CB	VAL	118	-2.062	-4.670	30.111	1.00	18.65
MOTA	573	CG1	L VAL	118	-0.804	-4.740	29.267	1.00	25.76
MOTA	574	CG2	VAL	118	-3.286	-4.556	29.217	1.00	16.20
MOTA	575	C	· VAL	118	-0.841	-6.136	31.744	1.00	19.05
MOTA	576	0	VAL	118	-0.680	-5.816	32.917	1.00	22.85
MOTA	577	N	THR	119	0.108	-6.726	31.023	1.00	17.25
MOTA	578	CA	THR	119	1.444	-6.962	31.546	1.00	18.76
MOTA	579	CB	THR	119	1.429	-8.081	32.623	1.00	18.92
ATOM	580	OG:	l THR	119	2.769	-8.438	32.995	1.00	6.16
MOTA	581	CG:	2 THR	119	0.670	-9.301	32.129	1.00	26.90
ATOM	582	C	THR	119	2.414	-7.273	30.406	1.00	19.69
MOTA	583	0	THR	119	2.474	-8.402	29.908	1.00	25.39
MOTA	584	N	HIS	120	3.170	-6.259	29.988	1.00	17.60
MOTA	585	CA	HIS	120	4.125	-6.423	28.888	1.00	8.64
MOTA	586	CB	HIS	120	3.359	-6.285	27.568	1.00	17.21
MOTA	587	CG	HIS	120	4.074	-6.841	26.371	1.00	16.80
MOTA	588	CD:	2 HIS	120	5.268	-6.531	25.816	1.00	19.94

#### FIG. 1K

MOTA	589	ND1	HIS	120	3.538	-7.834	25.585	1.00	14.74
ATOM	590	CE1	HIS	120	4.367	-8.115	24.598	1.00	13.09
ATOM	591	NE2	HIS	120	5.426	-7.338	24.717	1.00	15.49
ATOM	592	С	HIS	120	5.197	-5.346	28.996	1.00	2.84
ATOM	593	0	HIS	120	4.887	-4.197	29.245	1.00	2.73
ATOM	594	N	LYS	121	6.452	-5.709	28.750	1.00	2.00
ATOM	595	CA	LYS	121	7.568	-4.770	28.844	1.00	5.68
ATOM	596	CB	LYS	121	8.908	-5.490	28.616	1.00	6.54
ATOM	597	CG	LYS	121	9.144	-5.913	27.166	1.00	19.16
ATOM	598	CD	LYS	121	10.552	-6.453	26.901	1.00	25.40
ATOM	599	CE	LYS	121	11.608	-5.352	26.768	1.00	32.20
ATOM	600	NZ	LYS	121	12.953	-5.909	26.390	1.00	30.85
ATOM	601	C	LYS	121	7.477	-3.594	27.876	1.00	12.80
ATOM	602	ō	LYS	121	8.339	-2.714	27.883	1.00	18.97
ATOM	603	N	ASN	122	6.483	-3.613	26.995	1.00	15.97
ATOM	604	CA	ASN	122	6.310	-2.529	26.036	1.00	15.61
	605	CB	ASN	122	6.308	-3.077	24.602	1.00	22.61
MOTA	606	CG	ASN	122	7.577	-3.861	24.264	1.00	20.48
MOTA			ASN	122	7.516	-5.032	23.900	1.00	26.08
ATOM	607	ND2	ASN	122	8.732	-3.218	24.413	1.00	20.44
MOTA	608		ASN	122	5.024	-1.787	26.362	1.00	12.94
MOTA	609	C	ASN	122	4.501	-1.023	25.554	1.00	13.23
MOTA	610	0	ILE	123	4.521	-2.034	27.561	1.00	8.08
MOTA	611	N		123	3.325	-1.391	28.057	1.00	12.42
ATOM	612	CA	ILE	123	2.107	-2.339	28.020	1.00	11.96
ATOM	613	CB	ILE	123	0.891	-1.662	28.611	1.00	7.57
ATOM	614	CG2		123	1.805	-2.736	26.573	1.00	17.32
ATOM	615		ILE	123	1.385	-1.579	25.677	1.00	15.53
MOTA	616	CD1			3.623	-0.915	29.484	1.00	18.69
MOTA	617	C	ILE	123 123	4.462	-1.480	30.183	1.00	21.74
MOTA	618	0	ILE		2.966	0.164	29.895	1.00	22.62
ATOM	619	N	ILE	124	3.174	0.763	31.208	1.00	20.00
ATOM ·	620	CA	ILE	124	2.404	2.106	31.338	1.00	16.67
MOTA	621	CB	ILE	124	0.902	1.890	31.120	1.00	15.34
MOTA	622	CG2		124	2.694	2.740	32.699	1.00	7.20
MOTA	623	CG1		124	2.108	4.106	32.873	1.00	11.63
MOTA	624	CD1		124		-0.104	32.423	1.00	20.91
ATOM	625	C	ILE	124	2.853 1.765	-0.685	32.527	1.00	19.21
MOTA	626	0	ILE	124		-0.170	33.339	1.00	20.40
ATOM	627	N	SER	125	3.819	-0.917	34.594	1.00	19.59
MOTA	628	CA	SER	125	3.680	-1.974	34.750	1.00	23.73
MOTA	629	CB	SER	125	4.782	-1.375	34.987	1.00	31.90
MOTA	630	OG	SER	125	6.055	0.086	35.743	1.00	13.73
MOTA	631	C	SER	125	3.794	0.559	36.075	1.00	4.90
MOTA	632	0	SER	125	4.892 2.645	0.438	36.301	1.00	6.91
MOTA	633	N	LEU	126		1.368	37.409	1.00	7.11
MOTA	634	CA	LEU	126	2.578	1.807	37.607	1.00	2.00
MOTA	635	CB	LEU	126	1.128	3.295	37.543	1.00	2.00
ATOM	636	ICG	LEU	126	0.801	3.953	36.336	1.00	2.00
MOTA	637		r TEA	126	1.449		37.508	1.00	2.04
MOTA	638		5 TEA	126	-0.704	3.451		1.00	10.24
MOTA	639		LEU	126	3.108	0.694	38.689 39.112	1.00	10.24
MOTA	640		LEU	126	2.604	-0.345	39.112	1.00	11.75
MOTA	641		LEU	127	4.157	1.268		1.00	10.20
MOTA	642		ΓEÂ	127	4.751			1.00	
MOTA	643		LEU	127	6.199				
MOTA	644				7.253				
MOTA	645		1 LEU		8.601				
MOTA	646		2 ĻEU		7.278				_
MOTA	647	C	ĹEU	127	3.995	1.145	41.770	1.00	12.00

## FIG. 1L

MOTA	648	0	LEU	127	4.147	0.488	42.809	1.00	15.93
ATOM	649	N	ASN	128	3.192	2.209	41.704	1.00	14.08
MOTA	650	CA	ASN	128	2.460	2.679	42.883	1.00	14.71
MOTA	651	CB	ASN	128	3.473	3.186	43.923	1.00	17.09
ATOM	652	CG	ASN	128	2.868	3.398	45.299	1.00	18.33
MOTA	653	OD1	ASN	128	1.686	3.131	45.530	1.00	18.44
ATOM	654	ND2		128	3.686	3.875	46.228	1.00	15.54
ATOM	655		ASN	128	1.482	3.800	42.523	1.00	13.51
ATOM	656	0	ASN	128	1.805	4.674	41.735	1.00	17.61
ATOM	657	N	VAL	129	0.306	3.769	43.136	1.00	12.90
ATOM	658	CA	VAL	129	-0.753	4.754	42.935	1.00	15.50
ATOM	659	CB	VAL	129	-2.024	4.065	42.385	1.00	16.54
MOTA	660	CG1		129	-3.127	5.066	42.150	1.00	14.67
MOTA	661	CG2		129	-1.703	3.312	41.127	1.00	21.62
ATOM	662	C	VAL	129	-1.091	5.342	44.311	1.00	20.34
ATOM	663	ō	VAL	129	-1.519	4.607	45.206	1.00	22.82
MOTA	664	N	PHE	130	-0.928	6.653	44.494	1.00	22.42
ATOM	665	CA	PHE	130	-1.223	7.241	45.801	1.00	17.23
ATOM	666	CB	PHE	130	-0.026	7.082	46.727	1.00	9.18
ATOM	667	CG	PHE	130	1.126	7.968	46.380	1.00	3.29
ATOM	668		PHE	130	2.221	7.451	45.710	1.00	3.28
ATOM	669		PHE	130	1.129	9.309	46.753	1.00	2.00
MOTA	670		PHE	130	3.304	8.250	45.409	1.00	6.45
ATOM	671		PHE	130	2.201	10.125	46.461	1.00	2.00
ATOM	672	CZ	PHE	130	3.295	9.602	45.785	1.00	6.75
	673	C	PHE	130	-1.707	8.682	45.868	1.00	20.03
MOTA MOTA	674	0	PHE	130	-1.308	9.537	45.082	1.00	23.64
MOTA	675	И	THR	131	-2.511	8.949	46.892	1.00	20.98
	676	CA	THR	131	-3.068	10.269	47.129	1.00	16.85
MOTA	677	CB	THR	131	-4.611	10.245	47.082	1.00	11.46
MOTA	678	OG1		131	-5.132	11.530	47.426	1.00	11.14
MOTA	679	CG2		131	-5.163	9.211	48.031	1.00	7.42
MOTA	680	C	THR	131	-2.637	10.770	48.498	1.00	20.65
MOTA	681	0	THR	131	-2.667	10.026	49.474	1.00	25.07
MOTA	682	N	PRO	132	-2.151	12.016	48.569	1.00	21.95
MOTA	683	CD	PRO	132	-1.729	12.903	47.472	1.00	22.01
MOTA	684	CA	PRO	132	-1.733	12.554	49.868	1.00	20.75
MOTA	685	CB	PRO	132	-0.821	13.714	49.475	1.00	18.92
ATOM	686	CG	PRO	132	-1.429	14.194	48.195	1.00	22.75
MOTA		C	PRO	132	-2.944	12.996	50.709	1.00	19.68
ATOM	687	o	PRO	132	-2.797	13.419	51.852	1.00	24.00
MOTA	688 689	И	GLN	133	-4.142	12.878	50.146	1.00	17.03
MOTA	690	CA	GLN	133	-5.354	13.253	50.853	1.00	17.14
MOTA		CB	GLN	133	-6.425		49.892	1.00	16.91
ATOM	691		GLN	133	-6.158	15.188	49.391	1.00	10.35
ATOM	692	CG		133	-5.370	15.225	48.102	1.00	13.14
ATOM	693	CD	GLN GLN	133	-5.778	14.646	47.112	1.00	3.25
ATOM	694				-4.239	15.913	48.108	1.00	10.03
ATOM.	695		GLN	133	-5.864	12.064	51.657	1.00	21.25
ATOM	696	C	GLN	133	-5.723	10.910	51.239	1.00	22.26
ATOM	697	0	GLN	133	-6.449	12.353	52.815	1.00	22.44
ATOM	698	N	LYS	134	-6.939	11.318	53.709	1.00	25.31
ATOM	699	CA	LYS	134	-6.562	11.671	55.156	1.00	27.68
ATOM	700	CB	LYS	134	-5.241	11.048	55.621	1.00	33.88
ATOM	701		LYS	134	-3.241 -4.014	11.475	54.805		33.67
ATOM	702	CD	LYS	134	-3.590	12.911	55.101		36.64
ATOM	703		LYS	134		13.180	54.640		33.55
ATOM	704		LYS	134	-2.188	10.907			26.52
MOTA	705		LYS	134	-8.405	9.832			25.08
MOTA	706	0	LYS	134	-8.770	2.02	22.022		,_,



#### FIG. 1M

		•					-n 040	- 00	27 26
MOTA	707	N	THR	135	-9.252	11.755	53.042	1.00	27.26 29.66
MOTA	708	CA	THR	135	-10.666	11.416	52.896	1.00	31.92
MOTA	709	CB	THR	135	-11.543	12.164	53.913	1.00	
ATOM	710	OG1	THR	135	-11.281	13.570	53.829	1.00	37.53
MOTA	711	CG2	THR	135	-11.257	11.676	55.327	1.00	34.45
ATOM	712	С	THR	135	-11.214	11.685	51.499	1.00	30.80
MOTA	713	0	THR	135	-10.553	12.299	50.657	1.00	29.91
ATOM	714	N	LEU	136	-12.446	11.235	51.272	1.00	31.35
ATOM	715	CA	LEU	136	-13.120	11.414	49.994	1.00	30.05
ATOM	716	CB	LEU	136	-14.418	10.611	49.955	1.00	25.71
ATOM	717	CG	LEU	136	-15.412	10.924	48.833	1.00	21.56
ATOM	718	CD1	LEU	136	-14.746	10.754	47.477	1.00	20.38
ATOM	719	CD2	LEU	136	-16.627	10.026	48.961	1.00	19.40
MOTA	720	C	LEU	136	-13.402	12.883	49.707	1.00	33.09
ATOM	721	0	LEU	136	-13.129	13.352	48.607	1.00	34.24
ATOM	722	N	GLU	137	-13.943	13.603	50.692	1.00	34.66
ATOM	723	CA	GLU	137	-14.244	15.019	50.500	1.00	36.88
ATOM	724	CB	GLU	137	-15.090	15.597	51.651	1.00	40.97
ATOM	725	CG	GLU	137	-14.366	15.793	52.994	1.00	45.75
ATOM	726	CD	GLU	137	-14.984	16.907	53.855	1.00	49.12
ATOM	727		GLU	137	-14.225	17.783	54.330	1.00	48.83
ATOM	728		GLU	137	-16.221	16.911	54.055	1.00	46.20
ATOM	729	C	GLU	137	-12.963	15.818	50.338	1.00	34.88
	730	0	GLU	137	-12.927	16.808	49.613	1.00	37.49
MOTA	731	N	GLU	138	-11.904	15.372	50.996	1.00	32.51
ATOM	732	CA	GLU	138	-10.631	16.059	50.920	1.00	33.95
MOTA			GLU	138	-9.824	15.785	52.190	1.00	35.96
ATOM	733	CB CG	GLU	138	-8.508	16.532	52.268	1.00	38.62
ATOM	734	CD	GLU	138	-7.437	15.739	53.002	1.00	44.42
MOTA	735			138	-7.798	14.832	53.792	1.00	47.64
MOTA	736		GLU	138	-6.235	16.014	52.775	1.00	38.08
ATOM	737	OE2		138	-9.827	15.665	49.675	1.00	34.17
MOTA	738	C	GLU	138	-8.968	16.433	49.233	1.00	35.17
ATOM	739	0	GLU	139	-10.116	14.482	49.123	1.00	29.77
ATOM	740	N	PHE	139	-9.452	13.934	47.935	1.00	23.01
MOTA	741	CA	PHE		-10.202	12.694	47.459	1.00	17.20
ATOM	742	CB	PHE	139	-9.651	12.103	46.186	1.00	12.63
MOTA	743	CG	PHE	139	-8.285	11.903	46.033	1.00	10.00
MOTA	744		PHE	139	-10.500	11.781	45.128	1.00	7.51
ATOM	745		PHE	139		11.406	44.848	1.00	4.34
ATOM	746		PHE	139	-7.768	11.286	43.944	1.00	4.17
MOTA	747		PHE	139	-9.999	11.096	43.799	1.00	2.93
MOTA	748	CZ	PHE	139	-8.627	14.946	46.792	1.00	23.97
ATOM	749	С	PHE	139	-9.359	15.493	46.355	1.00	25.86
ATOM	750	0	PHE	139	-10.377		46.247	1.00	21.95
MOTA	751	N	GLN	140	-8.160	15.122	45.202	1.00	23.71
MOTA	752	CA	GLN	140	-7.928	16.114		1.00	25.69
MOTA	753	CB	GLN	140	-7.313	17.340	45.874		33.16
MOTA	754	CG	GLN	140	-6.997	18.504	44.998	1.00	36.46
ATOM	755	CD	GLN	140	-6.506	19.667	45.824	1.00	
MOTA	756	OE:	I GIN	140	-7.130	20.722	45.861	1.00	40.80
MOTA	757	NE	2 GLN	140	-5.402	19.464	46.533	1.00	36.20
MOTA	758	C	GLN	140	-7.035	15.631	44.052	1.00	22.46
MOTA	759	0	GLN	140	-7.459		42.898		24.38
MOTA	760	N	ASP	141	-5.806		44.383	•	19.44
ATOM	761	CA	ASP	141	-4.828		43.411		13.47
MOTA	762	CB	ASP	141	-3.531		43.626		13.18
MOTA	763	CG	ASP	141	-3.771		43.954		17.70
ATOM	764	OD:	1 ASP	141	-3.325		45.025		18.62
MOTA	765	OD:	2 ASP	141 .	-4.451	17.685	43.166	1.00	22.49

## FIG. 1N

ATOM	766	C	ASP	141	-4.529	13.290	43.472	1.00	15.68
MOTA	767	0	ASP	141	-4.865	12.607	44.441	1.00	15.84
MOTA	768	N	VAL	142	-3.912	12.785	42.406	1.00	17.48
ATOM	769	CA	VAL	142	-3.516	11.379	42.296	1.00	10.30
MOTA	770	CB	VAL	142	-4.422	10.604	41.327	1.00	6.58
MOTA	771	CG1	VAL	142	-3.933	9.181	41.198	1.00	5.29 6.09
ATOM	772	CG2	VAL	142	-5.873	10.648	41.798	1.00	
MOTA	773	C	VAL	142	-2.095	11.318	41.748	1.00	9.87
ATOM	774	0	VAL	142	-1.741	12.046	40.825	1.00	14.44 7.25
MOTA	775	N	TYR	143	-1.260	10.487	42.345	1.00	8.20
MOTA	776	CA	TYR	143	0.109	10.351	41.873	1.00	7.96
MOTA	777	CB	TYR	143	1.114	10.602	42.996	1.00 1.00	9.31
MOTA	778	CG	TYR	143	1.198	12.041	43.452	1.00	10.72
MOTA	779		TYR	143	0.144	12.645	44.136	1.00	14.58
MOTA	780		TYR	143	0.216	13.987	44.546 43.193	1.00	7.27
MOTA	781	CD2		143	2.332	12.809	43.193	1.00	9.99
MOTA	782	CE2		143	2.413	14.138		1.00	16.33
MOTA	783	$\mathbf{cz}$	TYR	143	1.352	14.725	44.273	1.00	17.53
ATOM	784	OH	TYR	143	1.442	16.047	44.664 41.335	1.00	12.96
ATOM	785	C	TYR	143	0.249	8.932	41.897	1.00	15.01
MOTA	786	0	TYR	143	-0.321	7.989	40.188	1.00	14.02
MOTA	787	N	LEU	144	0.916	8.807	39.530	1.00	6.63
MOTA	788	CA	LEU	144	1.143	7.520 7.521	38.147	1.00	3.96
MOTA	789	CB	LEU	144	0.498	7.521	38.041	1.00	7.52
MOTA	790	CG	LEU	144	-0.972	8.089	36.575	1.00	4.64
MOTA	791		LEU	144	-1.349	6.901	38.714	1.00	7.15
MOTA	792		LEU	144	-1.879 2.649	7.352	39.384	1.00	8.82
MOTA	793	C	LEU	144	3.327	8.239	38.857	1.00	8.56
MOTA	794	0	LEU	144	3.175	6.229	39.869	1.00	9.85
MOTA	795	N	VAL	145 145	4.614	5.965	39.804	1.00	10.26
ATOM	796	CA	VAL VAL	145	5.178	5.548	41.177	1.00	4.81
MOTA	797	CB CG1		145	6.701	5.576	41.147	1.00	2.00
ATOM	798 799	CG2		145	4.633	6.460	42.256	1.00	8.68
ATOM	800	C	VAL	145	4.896	4.889	38.769	1.00	10.28
MOTA	801	0	VAL	145	4.085	3.987	38.566	1.00	14.74
MOTA	802	N	MET	146	6.068	4.958	38.150	1.00	12.27
ATOM ATOM	803	CA	MET	146	6.443	4.025	37.085	1.00	13.67
ATOM	804	CB	MET	146	5.900	4.589	35.766	1.00	19.39
ATOM	805	CG	MET	146	5.719	3.620	34.624	1.00	28.14
MOTA	806	SD	MET	146	5.591	4.490	33.031	1.00	15.16
ATOM	807	CE	MET	146	7.177	4.095	32.403	1.00	11.15
MOTA	808	Ċ	MET	146	7.963	3.989	37.013	1.00	11.41
ATOM	809	ō	MET	146	8.638	4.765	37.681	1.00	14.24
ATOM	810	N	GLU	147	8.510	3.101	36.194	1.00	12.24
MOTA	811	CA	GLU	147	9.958	3.026	36.057	1.00	10.39
ATOM	812	СВ	GLU	147	10.359	1.764	35.301	1.00	13.37
ATOM	813	CG	GLU	147	11.869	1.594	35.228	1.00	20.29
ATOM	814	CD	GLU	147	12.306	0.436	34.356	1.00	20.99
ATOM	815		1 GLU	147	11.442	-0.188	33.700	1.00	21.78
ATOM	816	OE:		147	13.522	0.154	34.333	1.00	24.35
MOTA	817		GLU	147	10.446	4.260	35.296		7.60
ATOM	818		GLU	147	9.725	4.810			8.87
ATOM	819		LEU	148	11.678	4.673	35.552		
ATOM	820			148	12.229	5.851			
ATOM	821			148	13.273				
MOTA	822			148	13.777				
ATOM	823		1 LEU	148	12.635				
ATOM	824		2 LEU	148	14.917	8.373	36.224	1.00	2.00



#### FIG. 10

										_
MOTA	825	С	LEU	148		12.836	5.617	33.521	1.00	14.45
ATOM	826	0	LEU	148		13.896	4.986	33.382	1.00	10.38
MOTA	827	N	MET	149		12.190	6.207	32.516	1.00	20.38
ATOM	828	CA	MET	149		12.637	6.128	31.124	1.00	18.31
MOTA	829	CB	MET	149		11.440	5.978	30.181	1.00	15.17
ATOM	830	CG	MET	149	•	10.546	4.739	30.472	1.00	13.81
ATOM	831	SD	MET	149		11.392	3.117	30.550	1.00	14.34
MOTA	832	CE	MET	149		11.336	2.605	28.796	1.00	7.98
ATOM	833	C	MET	149		13.435	7.393	30.817	1.00	17.37
ATOM	834	0	MET	149		13.161	8.458	31.382	1.00	14.19
ATOM	835	N	ASP	150		14.432	7.255	29.946	1.00	18.71
ATOM	836	CA	ASP	150		15.335	8.347	29.569	1.00	19.67
ATOM	837	CB	ASP	150		16.615	7.768	28.963	1.00	20.46
ATOM	838	CG	ASP	150		17.313	6.786	29.887	1.00	25.54
ATOM	839	OD1	ASP	150		16.738	6.394	30.928	1.00	33.84
ATOM	840	OD2	ASP	150		18.455	6.398	29.572	1.00	29.63
MOTA	841	C	ASP	150		14.823	9.462	28.659	1.00	19.58
ATOM	842	Ō	ASP	150		15.312	10.595	28.742	1.00	19.97
MOTA	843	N	ALA	151		13.893	9.144	27.761	1.00	16.48
ATOM	844	CA	ALA	151		13.347	10.151	26.844	1.00	12.89
ATOM	845	СВ	ALA	151		14.307	10.386	25.668	1.00	13.41
ATOM	846	C	ALA	151		12.017	9.681	26.321	1.00	9.93
ATOM	847	ō	ALA	151		11.587	8.580	26.649	1.00	12.65
ATOM	848	N	ASN	152		11.309	10.555	25.615	1.00	6.98
ATOM	849	CA	ASN	152		10.053	10.144	25.019	1.00	14.22
ATOM	850	CB	ASN	152		8.881	11.095	25.325	1.00	15.50
ATOM	851	CG	ASN	152		9.113	12.510	24.852	1.00	22.15
ATOM	852		ASN	152		8.257.	13.092	24.180	1.00	22.15
MOTA	853		ASN	152		10.232	13.098	25.253	1.00	33.84
ATOM	854	С	ASN	152		10.349	10.018	23.535	1.00	19.02
ATOM	855	0	ASN	152		11.479	10.301	23.114	1.00	15.48
MOTA	856	N	LEU	153		9.365	9.577	22.750	1.00	19.93
MOTA	857	CA	LEU	153		9.561	9.371	21.316	1.00	15.53
MOTA	858	CB	LEU	153		8.370	8.655	20.694	1.00	11.21 8.57
MOTA	859	CG	LEU	153		8.669	7.298	20.059	1.00	3.71
MOTA	860	CD1	LEU	153		7.553	7.003	19.109	1.00	6.14
MOTA	861	CD2	LEU	153		10.003	7.285	19.322	1.00	15.22
MOTA	862	C	LEU	153		9.885	10.622	20.519	1.00	13.43
ATOM	863	0	LEU	153		10.859	10.635	19.777	1.00	15.83
MOTA	864	N	CYS	154		9.107	11.684	20.714	1.00 1.00	13.76
MOTA	865	CA	CYS	154		9.311	12.947	20.005		11.00
MOTA	866	CB	CYS	154		8.434	14.036	20.617 20.491	1.00	25.02
MOTA	867	਼ SG	CYS	154		6.668	13.722	20.491	1.00	11.62
MOTA	868	C	CYS	154		10.771	13.407		_	16.82
MOTA	869	0	CYS	154		11.220	14.080	19.085 21.037		13.05
MOTA	870	N	GLN	155		11.515	13.010	21.037		16.63
MOTA	871	CA	GLN	155		12.916	13.386	22.652		20.85
MOTA	872	CB	GLN	155		13.311	13.454	23.291		29.75
MOTA	873	ÇG	GLN	155		13.089	14.823	22.921		38.41
ATOM	874	CD		155		11.746	15.429			
MOTA	875		1 GLN	155		10.697	14.911	22.147		
ATOM	876			155		11.774	16.516			
MOTA	877		GLN	155		13.823	12.436 12.794			
MOTA	878		GLN	155		14.937	12.794			
MOTA	879		VAL	156		13.324	10.194			
ATOM	880			156		14.056 13.539	8.759			
ATOM	881			156		14.570	7.709			
MOTA	882		1 VAL	156		13.224	8.670			
MOTA	883	CG	2 VAL	156		17.224	2.070			



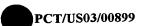
#### FIG. 1P

							4 = 0 = =	1 00	10 01
ATOM	884	C	VAL	156	13.833	10.457	17.977	1.00	10.81 10.61
ATOM	885	0	VAL	156	14.767	10.403	17.179	1.00	6.45
MOTA	886	N	ILE	157	12.607	10.838	17.628	1.00	8.99
MOTA	887	CA	ILE	157	12.221	11.141	16.260		2.57 .
MOTA	888	CB	ILE	157	10.785	11.690	16.217	1.00	2.00
ATOM	889	CG2	ILE	157	10.543	12.480	14.940	1.00	2.00
MOTA	890	CG1	ILE	157	9.795	10.541	16.387	1.00	2.00
ATOM	891	CD1	ILE	157	8.334	10.969	16.410	1.00	
ATOM	892	C	ILE	157	13.151	12.169	15.629	1.00	16.39 22.03
ATOM	893	0	ILE	157	13.500	12.066	14.451	1.00	
MOTA	894	N	GLN	158	13.563	13.158	16.411	1.00	16.88
ATOM	895	CA	GLN	158	14.439	14.183	15.882	1.00	19.76
ATOM	896	CB.	GLN	158	14.283	15.487	16.667	1.00	24.43
ATOM	897	CG	GLN	158	13.262	16.468	16.064	1.00	29.67
MOTA	898	CD	GLN	158	13.670	17.030	14.692	1.00	33.29
ATOM	899	OE1	GLN	158	14.844	16.990	14.293	1.00	32.74
MOTA	900	NE2	GLN	158	12.691	17.568	13.971	1.00	38.14
ATOM	901	С	GLN	158	15.898	13.787	15.773	1.00	21.28
ATOM	902	0	GLN	158	16.672	14.471	15.100	1.00	23.06
MOTA	903	N	MET	159	16.288	12.688	16.408	1.00	23.90
ATOM	904	CA	MET	159	17.679	12.256	16.333	1.00	27.52
ATOM	905	CB	MET	159 ·	18.105	11.504	17.594	1.00	26.97
ATOM	906	CG	MET	159	17.551	10.111	17.752	1.00	28.99
MOTA	907	SD	MET	159	17.963	9.398	19.365	1.00	33.77
ATOM	908	CE	MET	159	19.687	8.923	19.107	1.00	25.01
ATOM	909	C	MET	159	17.883	11.410	15.089	1.00	29.07
ATOM	910	0	MET	159	16.944	10.796	14.592	1.00	26.59
ATOM	911	N	GLU	160	19.096	11.440	14.549	1.00	33.57
ATOM	912	CA	GLU	160	19.416	10.686	13.344	1.00	37.97
ATOM	913	CB	GLU	160	20.781	11.117	12.803	1.00	43.50
MOTA	914	CG	GLU	160	21.038	10.753	11.353	1.00	48.38
ATOM	915	CD	GLU	160	22.314	11.387	10.826	1.00	54.65
ATOM	916	OE1	GLU	160	22.292	12.602	10.523	1.00	57.49
ATOM	917	OE2	GLU	160	23.340	10.678	10.726	1.00	58.34
ATOM	918	С	GLU	160	19.396	9.191	13.649	1.00	40.57
MOTA	919	0	GLU	160	20.360	8.622	14.180	1.00	41.54
ATOM	920	N	LEU	161	18.255	8.578	13.358	1.00	40.99
MOTA	921	CA	LEU	161	18.055	7.156	13.595	1.00	38.14
ATOM	922	CB	LEU	161	16.623	6.870	14.057	1.00	32.66
ATOM	923	CG	LEU	161	16.120	7.358	15.409	1.00	27.51
ATOM	924		LEU	161	14.610	7.176	15.456	1.00	21.09
ATOM	925	CD2	LEU	161	16.808	6.606	16.542	1.00	18.19
ATOM	926	С	LEU	161	18.320	6.326	12.352	1.00	37.38
ATOM	927	0	LEU	161	17.863	6.652	11.252	1.00	38.37
ATOM	928	N	ASP	162	19.081	5.257	12.542	1.00	34.91
ATOM	929	CA	ASP	162	19.373	4.343	11.463	1.00	32.15
ATOM	930	CB	ASP	162	20.738	3.675	11.661	1.00	31.54
ATOM	931	CG	ASP	162	20.992	3.253	13.092	1.00	23.98
ATOM	932		L ASP	162	22.164	3.334	13.510	1.00	24.51
ATOM	933		2 ASP	162	20.045	2.830	13.792	1.00	20.55
ATOM	934	С	ASP	162	18.259	3.311		1.00	30.83
ATOM	935	ō	ASP	162	17.355	3.354		1.00	30.69
ATOM	936		HIS	163	18.353			1.00	28.95
ATOM	937			163	17.344	1.321		1.00	24.49
ATOM	938			163	17.536			1.00	21.42
ATOM	939			163 .	17.233				14.24
ATOM	940		2 HIS	163	18.047				4.27
ATOM	941		1 HIS	163	15.944				10.79
ATOM	942		1 HIS	163	15.979	2.547	6.471	1.00	9.18
112011				-					



# FIG. 1Q

ATOM	943	NE2	HIS	163	17.242	2.720	6.122	1.00	9.38
MOTA	944	C	HIS	163	17.245	0.350	11.569	1.00	18.99 17.25
MOTA	945	0	HIS	163	16.146	0.003	11.988 12.131	1.00	16.05
MOTA	946	N	GLU	164	18.381	-0.040 -0.982	13.244	1.00	21.01
MOTA	947	CA	GLU	164	18.371		13.244	1.00	25.61
MOTA	948	CB	GLU	164	19.800	-1.348	12.549	1.00	42.31
ATOM	949	CG	GLU	164	20.871	-1.297	11.198	1.00	50.14
MOTA	950	CD	GLU	164	20.424	-1.884	11.151	1.00	53.63
MOTA	951	OE1		164	19.937	-3.038 -1.183	10.167	1.00	50.34
MOTA	952	OE2	GLU	164	20.576 17.575	-0.385	14.411	1.00	20.56
MOTA	953	C	GLU	164	16.705	-1.042	14.989	1.00	18.15
ATOM	954	0	GLU	164 165	17.816	0.893	14.689	1.00	20.23
MOTA	955	N	ARG ARG	165	17.123	1.597	15.755	1.00	16.22
ATOM	956	CA	ARG	165	17.782	2.948	16.028	1.00	18.25
ATOM	957	CB CG	ARG	165	18.675	2.981	17.264	1.00	20.28
ATOM	958	CD	ARG	165	19.244	4.370	17.508	1.00	21.80
MOTA	959	NE	ARG	165	20.669	4.460	17.180	1.00	31.00
ATOM	960 961	CZ	ARG	165	21.221	5.434	16.456	1.00	32.61
ATOM ATOM	962	NH1		165	20.470	6.416	15.969	1.00	33.22
ATOM	963	NH2		165	22.533	5.437	16.234	1.00	31.30
ATOM	964	C	ARG	165	15.651	1.811	15.433	1.00	16.58
ATOM	965	ō	ARG	165	14.793	1.606	16.290	1.00	20.41
ATOM	966	N	MET	166	15.351	2.186	14.192	1.00	13.52
ATOM	967	CA	MET	166	13.968	2.440	13.795	1.00	10.96
ATOM	968	CB	MET	166	13.900	3.213	12.477	1.00	16.45
MOTA	969	CG	MET	166	12.457	3.530	12.024	1.00	19.78
ATOM	970	SD	MET	166	12.325	4.695	10.654	1.00	7.28
ATOM	971	CE	MET	166	14.027	5.413	10.686	1.00	2.00
ATOM	972	C	MET	166	13.107	1.193	13.701	1.00	13.90
ATOM	973	0	MET	166	11.895	1.251	13.938	1.00	10.78
MOTA	974	N	SER	167	13.714	0.075	13.307	1.00	12.74
MOTA	975	CA	SER	167	12.972	-1.178	13.210	1.00	11.00
MOTA	976	CB	SER	167	13.730	-2.231	12.381	1.00	4.79
MOTA	977	OG	SER	167	15.127	-2.242	12.637	1.00	4.90
MOTA	978	С	SER	167	12.637	-1.700	14.600	1.00	8.72 9.37
MOTA	979	0	SER	167	11.505	-2.142	14.837	1.00	10.15
MOTA	980	N	TYR	168	13.595	-1.577	15.526	1.00 1.00	11.89
MOTA	981	CA	TYR	168	13.424	-2.019	16.918	1.00	13.12
MOTA	982	CB	TYR	168	14.710	-1.851	17.723 19.047	1.00	23.94
MOTA	983	CG	TYR	168	14.653	-2.568	19.047	1.00	27.00
MOTA	984	CD1		168	14.059	-3.823 -4.485	20.357	1.00	26.88
ATOM	985	CE1		168	13.986	-2.000	20.337	1.00	27.43
ATOM	986	CD2		168	15.177 15.105	-2.665	21.419	1.00	26.40
ATOM	987	CE2		168	14.505	-3.905	21.483	1.00	25.71
ATOM	988	CZ	TYR	168	14.410	-4.560		1.00	29.78
ATOM	989	ОН	TYR	168 168	12.309	-1.281	17.638	1.00	10.11
ATOM	990	C	TYR	168	11.514	-1.894	18.352	1.00	15.94
ATOM	991	0	TYR LEU	169	12.280	0.039	17.479	1.00	9.20
MOTA	992 993	N CA	LEU	169	11.250	0.870	18.083	1.00	6.55
MOTA MOTA	994	CB	LEU	169	11.512	2.365	17.796	1.00	5.56
MOTA	995	CG	LEU	169	12.697	3.034	18.506	1.00	2.00
	996		l LEU	169	12.942	4.395	17.946	1.00	2.00
ATOM ATOM	997		2 LEU	169	12.431	3.110	20.009	1.00	2.00
ATOM	998	CD.	LEU	169	9.896	0.464	17.526	1.00	8.60
ATOM	999	o	LEU	169	8.966	0.175	18.289	1.00	11.07
ATOM	1000	N	LEU	170	9.803	0.410	16.193	1.00	14.62
MOTA	1001	CA	LEU	170	8.563	0.035	15.516	1.00	13.43



#### FIG. 1R

										16 40
ATOM	1002	CB	LEU	170		8.679	0.192	13.992	1.00 1.00	16.49 8.13
MOTA	1003	CG	LEU	170		8.346	1.526	13.310	1.00	7.52
MOTA	1004	CD1		170		6.970	2.026	13.733	1.00	12.95
MOTA	1005		LEU	170		9.395	2.545	13.642	1.00	14.08
ATOM	1006	C	LEU	170		8.155	-1.393	15.868 15.974	1.00	16.12
MOTA	1007	0	LEU	170		6.963	-1.695	16.098	1.00	14.62
MOTA	1008	N	TYR	171		9.139	-2.260	16.471	1.00	15.32
MOTA	1009	CA	TYR	171		8.860	-3.642	16.498	1.00	20.86
MOTA	1010	CB	TYR	171		10.156	-4.453 -5.803	17.174	1.00	30.51
ATOM	1011	CG	TYR	171		10.039	-6.821	16.634	1.00	29.52
MOTA	1012	CD1	TYR	171		9.248 9.120	-8.046	17.282	1.00	35.08
ATOM	1013	CE1	TYR	171		10.701	-6.054	18.375	1.00	29.23
MOTA	1014	CD2	TYR	171		10.701	-7.272	19.022	1.00	31.42
MOTA	1015	CE2	TYR	171		9.786	-8.262	18.477	1.00	34.50
MOTA	1016	CZ	TYR	171 171		9.665	-9.464	19.133	1.00	35.71
MOTA	1017	OH	TYR	171		8.174	-3.685	17.842	1.00	16.71
ATOM	1018	C	TYR TYR	171		7.111	-4.302	17.999	1.00	22.65
MOTA	1019	0	GLN	172		8.759	-2.993	18.820	1.00	12.16
MOTA	1020	N CA	GLN	172		8.207	-2.953	20.174	1.00	8.36
MOTA	1021	CB	GLM	172		9.174	-2.245	21.100	1.00	7.90
MOTA	1022 1023	CG	GLN	172		10.537	-2.885	21.101	1.00	9.40
MOTA	1023	CD	GLN	172		11.522	-2.124	21.942	1.00	16.58
MOTA	1024		GLN	172		11.507	-2.214	23.169	1.00	25.77
MOTA	1025	NE2		172		12.382	-1.362	21.292	1.00	14.95
ATOM ATOM	1027	C	GLN	172		6.836	-2.305	20.237	1.00	6.06
MOTA	1028	ō	GLN	172		5.990	-2.708	21.029	1.00	10.45
MOTA	1029	N	MET	173		6.607	-1.320	19.378	1.00	3.68
ATOM	1030	CA	MET	173		5.333	-0.635	19.332	1.00	2.37
ATOM	1031	CB	MET	173		5.400	0.520	18.335	1.00	10.38
MOTA	1032	CG	MET	173		5.939	1.827	18.917	1.00	14.77
ATOM	1033	SD	MET	173		5.978	3.168	17.706	1.00	15.09
ATOM	1034	CE	MET	173		7.699	3.414	17.615	1.00	2.00
MOTA	1035	C	MET	173		4.246	-1.615	18.940	1.00	4.64
MOTA	1036	0	MET	173	1	3.129	-1.572	19.462	1.00	2.00
ATOM	1037	N	LEU	174		4.603	-2.534	18.046	1.00	9.41
MOTA	1038	CA	LEU	174		3.672	-3.558	17.564	1.00	7.13 10.84
MOTA	1039	CB	LEU	174		4.151	-4.138	16.220	1.00	2.68
MOTA	1040	CG	LEU	174		4.139	-3.195	14.996	1.00	5.45
MOTA	1041	CD1		174		5.143	-3.637	13.942	1.00 1.00	2.00
MOTA	1042	CD2		174		2.752	-3.118	14.396 18.619	1.00	3.27
ATOM	1043	C	LEU	174		3.420	-4.647	18.825	1.00	2.00
MOTA	1044	0	LEU	174		2.272	-5.064	19.299	1.00	8.94
MOTA	1045	N	CYS	175		4.476		20.363	1.00	5.39
MOTA	1046	CA	CYS	175		4.325	-6.099 -6.386	21.040	1.00	2.00
MOTA	1047	CB	CYS	175		5.656		20.062		9.71
MOTA	1048	SG	CYS	175		6.885	-7.180 -5.518	21.420	_	8.35
MOTA	1049	C	CYS	175		3.385 2.448		21.872		9.82
MOTA	1050	0	CYS	175		3.630	-4.253	21.781		5.95
MOTA	1051	N	GLY	176		2.813		22.763		2.00
MOTA	1052		GLY	176		1.347				5.44
MOTA	1053	C	GLY	176 176		0.489				4.70
MOTA	1054	O	GLY	177		1.059				8.52
MOTA	1055		ILE	177		-0.321				9.46
MOTA	1056		ILE	177		-0.377				10.93
MOTA	1057			177		-1.791				13.45
MOTA	1058 1059		l ILE	177		0.484		_		6.12
MOTA MOTA	1060		1 ILE	177		0.672				12.58
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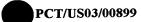


#### FIG. 1S

ATOM	1061	С	ILE	177	-0.984	-4.425	20.422	1.00	9.48
ATOM	1062	0	ILE	177	-2.202	-4.583	20.610	1.00	2.00
ATOM	1063	N	LYS	178	-0.193	-5.424	20.054	1.00	8.60
ATOM	1064	CA	LYS	178	-0.748	-6.757	19.877	1.00	13.96
ATOM	1065	CB	LYS	178	0.275	-7.712	19.247	1.00	11.31
ATOM	1066	CG	LYS	178	-0.280	-9.093	19.037	1.00	8.75
MOTA	1067	CD	LYS	178	0.682	-9.999	18.302	1.00	13.40
MOTA	1068	CE	LYS	178		-11.436	18.309	1.00	6.81
ATOM	1069	NZ	LYS	178		-11.536	18.017	1.00	8.76
ATOM	1070	C	LYS	178	-1.197	-7.236	21.261	1.00	12.95
ATOM	1071	0	LYS	178	-2.297	-7.773	21.406	1.00	11.31
ATOM	1072	N	HIS	179	-0.382	-6.959	22.282	1.00	14.07
ATOM	1072	CA	HIS	179	-0.720	-7.337	23.654	1.00	17.66
	1073	CB	HIS	179	0.411	-6.956	24.608	1.00	22.96
MOTA	1074	CG	HIS	179	0.252	-7.521	25.989	1.00	25.68
MOTA			HIS	179	-0.527	-7.144	27.031	1.00	21.69
ATOM	1076		HIS	179	0.975	-8.606	26.430	1.00	27.24
ATOM	1077			179	0.653	-8.874	27.681	1.00	25.21
ATOM	1078		HIS		-0.258	-8.002	28.067	1.00	25.80
ATOM	1079		HIS	179		-6.641	24.098	1.00	18.55
ATOM	1080	C	HIS	179	-2.010	-7.257	24.707	1.00	20.15
MOTA	1081	0	HIS	179	-2.891		23.766	1.00	19.43
ATOM	1082	N	LEU	180	-2.130	-5.360 4.570	24.125	1.00	18.86
ATOM	1083	CA	LEU	180	-3.302	-4.570		1.00	18.87
ATOM	1084	CB	LEU	180	-3.061	-3.092	23.792	1.00	17.95
MOTA	1085	CG	LEU	180	-3.163	-2.022	24.885	1.00	16.08
MOTA	1086		LEU	180	-2.288	-2.388	26.063		
MOTA	1087		LEU	180	-2.739	-0.672	24.323	1.00	19.02 17.60
MOTA	1088	С	LEU	180	-4.543	-5.075	23.400	1.00	
MOTA	1089	0	LEU	180	-5.638	-5.078	23.966	1.00	16.24
MOTA	1090	N	HIS	181	-4.370	-5.498	22.148	1.00	18.47
MOTA	1091	CA	HIS	181	-5.476	-6.016	21.346	1.00	18.34
MOTA	1092	CB	HIS	181	-5.058	-6.209	19.888	1.00	22.03
ATOM	1093	CG	HIS	181	-5.010	-4.939	19.094	1.00	24.29
MOTA	1094		HIS	181	-5.866	-3.896	19.030	1.00	22.97
MOTA	1095		HIS	181	-3.972	-4.639	18.238	1.00	23.58
MOTA	1096		HIS	181	-4.194	-3.462	17.681	1.00	20.84
MOTA	1097		HIS	181	-5.335	-2.989	18.145	1.00	21.33
ATOM	1098	C	HIS	181	-5.947	-7.338	21.914	1.00	14.91
MOTA.	1099	0	HIS	181	-7.142	-7.629	21.911	1.00	16.18
MOTA	1100	N	SER	182	-4.999	-8.127	22.413	1.00	16.17
MOTA	1101	CA	SER	182	-5.291	-9.425	23.011	1.00	16.47
MOTA	1102	CB	SER	182		-10.157	23.351	1.00	12.75
MOTA	1103	OG	SER	182		-10.271	22.215	1.00	23.12
MOTA	1104	C	SER	182		-9.200	24.288		18.77
ATOM	1105	0	SER	182	-6.934	-10.024	,24.661	1.00	24.36
MOTA	1106	N	ALA	183	-5.828	-8.070		1.00	17.65
MOTA	1107	CA	ALA	183	-6.506	-7.705	26.182	1.00	13.29
MOTA	1108	CB	ALA	183	-5.699	-6.670	26.919	1.00	13.15
MOTA	1109	C	ALA	183	-7.911	-7.183	25.911	1.00	16.33
ATOM	1110	0	ALA	183	-8.731	-7.066	26.826	1.00	22.38
ATOM	1111	N	GLY	184	-8.189	-6.883	24.646	1.00	16.47
ATOM	1112	CA	GLY	184	-9.490	-6.371	24.257	1.00	12.73
ATOM	1113	C	GLY	184	-9.461	-4.861	24.168	1.00	13.71
ATOM	1114	ō	GLY		-10.503		24.060	1.00	14.57
ATOM	1115	N	ILE	185	-8.256		24.189	1.00	14.45
ATOM	1116	CA	ILE	185	-8.047		24.141	1.00	17.69
ATOM	1117	CB	ILE	185	-7.032		25.266	1.00	14.32
ATOM	1118		ILE	185	-6.662		25.131	1.00	9.43
ATOM	1119		ILE	185	-7.635		26.650	1.00	12.09
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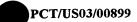
# FIG. 1T

ATOM	1120	CD1	ILE	185	-6.617	-2.904	27.750	1.00	2.00
ATOM	1121	C	ILE	185	-7.555	-2.353	22.780	1.00	21.86
MOTA	1122	0	ILE	185	-6.458	-2.706	22.336	1.00	23.69
ATOM	1123	N	ILE	186	-8.401	-1.588	22.089	1.00	23.04
MOTA	1124	CA	ILE	186	-8.006	-0.998	20.810	1.00	22.05
MOTA	1125	CB	ILE	186	-9.023	-1.248	19.666	1.00	22.99
ATOM	1126	CG2	ILE	186	-8.419	-0.786	18.345	1.00	19.01
MOTA	1127	CG1	ILE	186	-9.340	-2.743	19.553	1.00	20.59
MOTA	1128	CD1	ILE	186	-10.411	-3.065	18.541	1.00	15.12
MOTA	1129	С	ILE	186	-7.832	0.503	21.068	1.00	18.01
MOTA	1130	0	ILE	186	-8.794	1.248	21.280	1.00	19.97
MOTA	1131	N	HIS	187	-6.572	0.906	21.059	1.00	11.89 9.65
MOTA	1132	CA	HIS	187	-6.143	2.266	21.331	1.00	7.84
MOTA	1133	CB	HIS	187	-4.662	2.352	21.011	1.00	10.36
ATOM	1134	CG	HIS	187	-3.903	3.274	21.898	1.00	11.24
MOTA	1135		HIS	187	-4.054	4.595	22.156	1.00	
ATOM	1136	ND1	HIS	187	-2.778	2.877	22.586	1.00	13.01
MOTA	1137	CE1	HIS	187	-2.263	3.912	23.218	1.00	12.92
MOTA	1138	NE2	HIS	187	-3.015	4.964	22.975	1.00	4.76
MOTA	1139	C	HIS	187	-6.908	3.428	20.691	1.00	11.30 13.83
ATOM	1140	0	HIS	187	-7.731	4.064	21.348	1.00	14.27
ATOM	1141	N	ARG	188	-6.606	3.708	19.423	1.00 1.00	13.77
MOTA	1142	CA	ARG	188	-7.211	4.792	18.648		13.60
MOTA	1143	CB	ARG	188	-8.724	4.854	18.845	1.00	10.20
MOTA	1144	CG	ARG	188	-9.457	3.753	18.170	1.00	17.16
MOTA	1145	CD	ARG	188	-10.493	3.222	19.085	1.00	16.20
MOTA	1146	NE	ARG	188	-11.632	4.112	19.212	1.00 1.00	22.11
MOTA	1147	$\mathbf{cz}$	ARG	188	-12.508	4.040	20.206	1.00	22.61
MOTA	1148		ARG	188	-12.349	3.127	21.157	1.00	21.57
MOTA	1149		ARG	188	-13.576	4.829	20.218	1.00	17.28
MOTA	1150	С	ARG	188	-6.623	6.181	18.889	1.00	21.13
MOTA	1151	0	ARG	188	-7.229	7.173	18.501	1.00	15.55
MOTA	1152	N	ASP	189	-5.444	6.264	19.502	1.00	15.15
MOTA	1153	CA	ASP	189	-4.843	7.563	19.762 20.894	1.00	17.43
ATOM	1154	CB	ASP	189	-5.601	8.256		1.00	29.44
MOTA	1155	CG	ASP	189	-5.499	9.768	20.831	1.00	36.43
MOTA	1156		ASP	189	-5.155	10.316	19.759 21.861	1.00	39.38
MOTA	1157		ASP	189	-5.778	10.415		1.00	15.20
MOTA	1158	С	ASP	189	-3.361	7.474	20.087	1.00	16.94
MOTA	1159	0	ASP	189	-2.882	8.081	21.034 19.255	1.00	16.38
MOTA	1160	N	LEU	190	-2.632	6.747	19.255	1.00	14.72
MOTA	1161	CA	LEU	190	-1.205	6.553		1.00	17.54
MOTA	1162	CB	LEU	190	-0.753	5.278	18.741 19.644	1.00	12.34
MOTA	1163	CG	LEU	190	-0.255	4.158	18.825	1.00	12.26
ATOM	1164		LEU	190	0.027	2.938	20.360	1.00	13.72
MOTA	1165		FER TER	190	1.003	4.602	18.995	1.00	15.73
ATOM	1166	С	LEU	190	-0.350	7.723	17.805	1.00	20.11
MOTA	1167	0	LEU	190	-0.118	7.906		1.00	16.43
MOTA	1168	N	LYS	191	0.098	8.527	19.954 19.663	1.00	11.18
MOTA	1169	CA	LYS	191	0.956	9.675	20.051	1.00	15.07
MOTA	1170		LYS	191	0.259			1.00	17.28
MOTA	1171		LYS	191	-0.201		21.516 21.765		10.02
MOTA	1172		LYS	191	-1.088				14.89
MOTA	1173		LYS	191	-2.531				18.00
MOTA	1174		LYS	191	-3.522				10.22
MOTA	1175		LYS	191	2.279		_		16.35
ATOM	1176		LYS	191	2.312				
MOTA	1177		PRO	192	3.393				2.00
MOTA	1178	CD	PRO	192	3.460	10.575	10.433		2.00



#### FIG. 1U

ATOM	1179	CA	PRO	192	4.741	9.818	20.389	1.00	8.49
MOTA	1180	CB	PRO	192	5.612	10.513	19.342	1.00	9.05
MOTA	1181	CG	PRO	192	4.880	10.296	18.077	1.00	5.94
ATOM	1182	C	PRO	192	4.948	10.467	21.776	1.00	14.51
MOTA	1183	0	PRO	192	5.980	10.251	22.435	1.00	16.54
MOTA	1184	N	SER	193	3.991	11.294	22.192	1.00	13.30
ATOM	1185	CA	SER	193	4.051	11.984	23.473	1.00	14.80
ATOM	1186	CB	SER	193	3.120	13.207	23.461	1.00	14.49
MOTA	1187	OG	SER	193	1.785	12.862	23.103	1.00	8.59
MOTA	1188	С	SER	193	3.678	11.048	24.610	1.00	17.21 21.39
MOTA	1189	0	SER	193	4.047	11.279	25.763	1.00	15.65
MOTA	1190	N	ASN	194	2.938	9.999	24.258	1.00° 1.00	7.21
MOTA	1191	CA	ASN	194	2.482	8.981	25.192		7.21
AŢOM	1192	CB	ASN	194	1.043	8.593	24.865	1.00 1.00	21.77
MOTA	1193	CG	ASN	194	0.054	9.693	25.189	1.00	29.51
MOTA	1194		ASN	194	0.331	10.557	26.021 24.561	1.00	18.85
MOTA	1195		ASN	194	-1.118	9.658		1.00	6.70
MOTA	1196	C.		194	3.371	7.742 6.651	25.091 25.476	1.00	8.40
ATOM	1197	0	ASN	194	2.964 4.580	7.908	24.564	1.00	2.00
MOTA	1198	N	ILE	195		6.798	24.304	1.00	2.73
MOTA	1199	CA	ILE	195	5.507	6.355	22.899	1.00	5.68
ATOM	1200	CB	ILE	195	5.625 6.725	5.321	22.732	1.00	2.00
MOTA	1201	CG2	ILE	195 195	4.295	5.789	22.397	1.00	2.00
ATOM	1202	CG1			4.313	5.374	20.938	1.00	6.01
ATOM	1203	CD1	ILE ILE	195 195	6.858	7.244	24.903	1.00	3.99
ATOM	1204	0	ILE	195	7.315	8.341	24.584	1.00	8.39
MOTA	1205	И	VAL	196	7.500	6.375	25.676	1.00	5.82
MOTA	1206 1207	CA	VAL	196	8.803	6.663	26.270	1.00	11.18
MOTA MOTA	1207	CB	VAL	196	8.682	6.901	27.805	1.00	13.47
ATOM	1208		VAL	196	8.198	8.316	28.079	1.00	10.74
ATOM	1210	CG2		196	7.692	5.913	28.430	1.00	14.45
ATOM	1211	C	VAL	196	9.829	5.574	25.971	1.00	10.32
ATOM	1212	ō	VAL	196	9.479	4.403	25.825	1.00	21.42
ATOM	1213	N	VAL	197	11.089	5.971	25.808	1.00	5.51
ATOM	1214	CA	VAL	197	12.158	5.027	25.502	1.00	4.80
ATOM	1215	CB	VAL	197	12.639	5.133	24.002	1.00	10.58
ATOM	1216	·CG1		197	11.531	5.695	23.102	1.00	6.44
ATOM	1217	CG2		197	13.920	5.945	23.856	1.00	4.90
ATOM	1218	C	VAL	197	13.334	5.191	26.454	1.00	7.69
ATOM	1219	0	VAL	197	13.406	6.158	27.209	1.00	10.91
MOTA	1220	N	LYS	198	14.270	4.250	26.390	1.00	10.12
MOTA	1221	CA	LYS	198	15.442	4.243	27.254	1.00	11.52
MOTA	1222	CB	LYS	198	15.386	3.003	28.149	1.00	16.60
ATOM	1223	CG	LYS	198	16.189	3.136	29.427	1.00	26.28
MOTA	1224	CD	LYS	198	16.150	1.878	30.272	1.00	31.00
MOTA	1225	CE	LYS	198	14.768	1.615	30.854	1.00	37.45
ATOM	1226	NZ	LYS	198	14.780	0.433	31.779	1.00	39.49
MOTA	1227	C	LYS	198	16.712	4.240	26.403	1.00	16.21
MOTA	1228	0	LYS	198	16.637	4.095	25.187	1.00	17.79
ATOM	1229	N	SER	199	17.876	4.367	27.040	1.00	17.91
MOTA	1230	CA	SER	199	19.152	4.397	26.328	1.00	18.09
MOTA	1231	CB	SER		20.308	4.677	27.280	1.00	17.32 22.33
MOTA	1232	OG	SER		20.405	6.068	27.526	1.00	20.05
MOTA	1233	C	SER		19.475	3.190	25.447 24.548	1.00	20.03
MOTA	1234	0	SER		20.301	3.285	24.548	1.00	21.10
ATOM	1235	N	ASP	200	18.864	2.045	25.727	1.00	17.62
MOTA	1236	CA	ASP	200	19.086	0.872	25.724	1.00	14.14
MOTA	1237	CB	ASP	200	19.288	-0.408	23.124	1.00	T4.74



# FIG. 1V

MOTA	1238	CG	ASP	200		18.209	-0.625	26.779	1.00	13.05
ATOM	1239	OD1		200		17.051	-0.223	26.574	1.00	10.97
MOTA	1240	OD2	ASP	200		18.528	-1.231	27.822	1.00	13.20
MOTA	1241	C	ASP	200		17.875	0.776	23.977	1.00	18.24
MOTA	1242	0	ASP	200		17.465	-0.298	23.559	1.00	22.86 18.66
MOTA	1243	N	CYS	201		17.283	1.936	23.723	1.00	21.37
ATOM	1244	CA	CYS	201		16.114	2.071	22.870	1.00	22.84
MOTA	1245	CB	CYS	201		16.491	1.963	21.378	1.00	22.39
MOTA	1246	SG	CYS	201		17.104	3.519	20.591	1.00	20.00
MOTA	1247	C	CYS	201		14.929	1.170	23.205	1.00	25.61
ATOM	1248	0	CYS	201		14.077	0.934	22.347 24.437	1.00	15.48
MOTA	1249	N	THR	202		14.862	0.658		1.00	15.71
MOTA	1250	CA	THR	202		13.715	-0.174	24.815 26.087	1.00	15.14
MOTA	1251	CB	THR	202		13.954	-0.996	27.107	1.00	24.66
MOTA	1252	OG1	THR	202		14.531	-0.171	25.780	1.00	16.97
ATOM	1253	CG2	THR	202		14.881	-2.163	24.963	1.00	12.64
MOTA	1254	C	THR	202		12.539	0.772	25.454	1.00	18.75
MOTA	1255	0	THR	202		12.694	1.884	24.513	1.00	11.71
MOTA	1256	N	LEU	203		11.370	0.343	24.513	1.00	11.07
ATOM	1257	CA	LEU	203		10.192	1.202	23.035	1.00	7.87
ATOM	1258	CB	LEU	203		9.790	1.396 2.108	22.503	1.00	8.82
MOTA	1259	CG	LEU	203		8.550	2.537	21.066	1.00	6.21
MOTA	1260		LEU	203		8.821	1.200	22.578	1.00	2.00
MOTA	1261		LEU	203		7.330	0.752	25.339	1.00	12.47
MOTA	. 1262	C	LEU	203		8.994	-0.436	25.628	1.00	17.72
MOTA	1263	0	LEU	203		8.834	1.720	25.668	1.00	3.95
MOTA	1264	N	LYS	204	,	8.134 6.923	1.496	26.443	1.00	2.00
MOTA	1265	CA	LYS	204			1.693	27.944	1.00	3.61
ATOM	1266	CB	LYS	204		7.184 7.814	0.487	28.650	1.00	6.82
MOTA	1267	CG	LYS	204		8.128	0.807	30.098	1.00	8.75
MOTA	1268	CD	LYS	204		9.139	-0.175	30.683	1.00	10.28
ATOM	1269	CE	LYS	204 204		8.520	-1.437	31.124	1.00	8.47
ATOM	1270	NZ	LYS	204		5.854	2.477	25.996	1.00	2.00
MOTA	1271	C	LYS LYS	204		6.154	3.620	25.687	1.00	3.81
ATOM	1272	0	ILE	205		4.617	2.007	25.921	1.00	2.00
ATOM	1273	N	ILE	205		3.479	2.830	25.538	1.00	3.79
ATOM	1274	CA CB	ILE	205		2.498	2.070	24.610	1.00	6.77
ATOM	1275	CG2		205		1.214	2.877	24.403	1.00	2.00
MOTA	1276	CG2		205		3.167	1.763	23.270	1.00	7.79
ATOM	1277 1278	CD		205		2.238	1.080	22.284	1.00	7.74
ATOM ATOM	1279	CD.	ILE	205		2.751	3.138	26.834	1.00	11.47
ATOM	1280	Õ	ILE	205		2.189	2.244	27.462	1.00	13.38
	1281	N	LEU	206		2.667	4.418	27.165	1.00	12.52
ATOM	1282	CA	LEU	206		2.048	4.852	28.401	1.00	13.05
ATOM ATOM	1283	CB		206		. 2.527	6.264	28.749	1.00	15.77
MOTA	1284	CG		206 <sup>.</sup>		4.040		28.734	1.00	16.73
	1285		1 LEU	206		4.274		28.716	1.00	17.19
MOTA MOTA	1285		2 LEU	206		4.747		29.918	1.00	14.95
ATOM	1287	C	LEU	206		0.536			1.00	14.20
ATOM	1288	ō	LEU	206		0.064	4.541	29.655	1.00	19.67
ATOM	1289		ASP	207		-0.236	_	27.462	1.00	10.78
ATOM	1290			207		-1.692		27.636		10.76
ATOM	1291			207		-2.280				14.80
ATOM	1292			207		-2.281				22.89
ATOM	1293		1 ASP	207		-3.373				22.44
MOTA	1294		2 ASP	207		-1.204	6.511			
ATOM	1295		ASP	207		-2.507				
ATOM	1296		ASP	207		-1.956	2.926	26.223	1.00	15.31



#### FIG. 1W

ATOM	1297	N	PHE	208	-3.819	3.776	27.179	1.00	7.76
ATOM	1298	CA	PHE	208	-4.739	2.809	26.593	1.00	7.38
ATOM	1299	CB	PHE	208	-5.458	2.005	27.688	1.00	12.69
MOTA	1300	CG	PHE	208	-4.514	1.331	28.648	1.00	11.63
MOTA	1301	CD1	PHE	208	-4.326	1.833	29.932	1.00	19.85
MOTA	1302		PHE	208	-3.753	0.251	28.240	1.00	12.07
MOTA	1303	CE1	PHE	208	-3.368	1.269	30.793	1.00	16.31
MOTA	1304	CE2	PHE	208	-2.797	-0.323	29.080	1.00	14.94
MOTA	1305	CZ	PHE	208	-2.600	0.190	30.363	1.00	14.41
MOTA	1306	С	PHE	208	-5.738	3.488	25.669	1.00	10.81 7.83
ATOM	.1307	0	PHE	208	-6.769	2.917	25.326	1.00	
ATOM	1308	N	GLY	209	-5.457	4.749	25.345	1.00	14.37
MOTA	1309	CA	GLY	209	-6.269	5.515	24.414	1.00	11.22
ATOM	1310	C	GLY	209	-7.711	5.857	24.716	1.00	14.15
MOTA	1311	0	GLY	209	-8.073	6.130	25.864	1.00	16.16
MOTA	1312	N	LEU	210	-8.530	5.835	23.661	1.00	15.03
MOTA	1313	CA	LEU	210	-9.958	6.173	23.725	1.00	19.13
ATOM	1314	CB	LEU	210	-10.429	6.677	22.362	1.00	18.59
MOTA	1315	CG	LEU	210	-9.546	7.639	21.575	1.00	21.21
ATOM	1316	CD1	LEU	210	-10.096	7.786	20.162	1.00	21.04
MOTA	1317	CD2	LEU	210	-9.479	8.981	22.283	1.00	21.95
ATOM	1318	C	LEU	210	-10.895	5.048	24.140	1.00	23.06
ATOM	1319	0	LEU	210	-10.631	3.871	23.886	1.00	27.54
ATOM	1320	N	ALA	211	-12.023	5.428	24.730	1.00	26.46
MOTA	1321	CA	ALA	211	-13.029	4.460	25.152	1.00	31.93 33.70
ATOM	1322	CB	ALA	211	-13.833	5.013	26.324	1.00	
ATOM	1323	С	ALA	211	-13.938	4.200	23.954	1.00	37.57
MOTA	1324	0	ALA	211	-14.160	5.102	23.140	1.00	39.41
MOTA	1325	N	ALA	212	-14.456	2.975	23.848	1.00	41.47
MOTA	1326	CA	ALA	212	-15.334	2.574	22.741	1.00	44.00
MOTA	1327	CB	ALA	212	-15.865	1.170	22.987	1.00	40.73 46.85
MOTA	1328	С	ALA	212	-16.494	3.539	22.457	1.00	
MOTA	1329	0	ALA	212	-16.590	4.009	21.294	1.00	45.16 38.33
MOTA	1330	CB	VAL	225	-9.000	18.138	19.811	1.00	36.84
ATOM	1331		. VAL	225	-8.808	16.791	20.485	1.00	33.61
MOTA	1332	CG2	VAL	225	-10.183	18.882	20.426	1.00	46.33
MOTA	1333	C	VAL	225	-6.661	18.403	18.962	1.00	51.16
MOTA	1334	0	VAL	225	-6.466	18.939	17.870	1.00	45.47
MOTA	1335	N	VAL	225	-7.928	20.395	19.562	1.00	
MOTA	1336	CA	VAL	225	-7.699	18.972	19.928	1.00	42.53 47.37
ATOM	1337	N	THR	226	-5.978	17.340	19.378	1.00	43.20
MOTA	1338	CA	THR	226	-4.959	16.692	18.550	1.00	45.47
MOTA	1339	CB	THR	226	-3.798	16.159	19.417	1.00	44.76
MOTA	1340	OG1	LTHR	226	-3.273	17.220	20.231	1.00 1.00	41.66
MOTA	1341	CG2	2 THR	226	-2.690	15.583	18.538	1.00	41.24
MOTA	1342	C	THR	226	-5.544	15.517	17.770	1.00	41.37
MOTA	1343	0	THR	226	-6.141	14.608	18.355		37.27
ATOM	1344	N	ALA	227	-5.360	15.533	16.455	1.00	31.23
MOTA	1345	CA	ALA	227	-5.862	14.461	15.610	1.00	23.57
MOTA	1346	CB	ALA	227	-7.220	14.841	15.019	1.00	27.64
MOTA	1347	C	ALA	227	-4.868	14.132	14.500	1.00 1.00	30.70
MOTA	1348	0	ALA	227	-5.232	13.478	13.526		24.30
MOTA	1349	N	TYR	228	-3.612	14.552		1.00	23.17
MOTA	1350	CA		228	-2.575	14.312		1.00	
ATOM	1351			228	-1.246	14.990		1.00	
MOTA	1352			228	-1.291	16.467	_	1.00	
ATOM	1353		1 TYR	228	-0.197	17.108		1.00	
MOTA	1354		1 TYR	228	-0.219	18.457			
MOTA	1355	CD	2 TYR	228	-2.416	17.229	13.991	1.00	22.09

#### FIG. 1X

MOTA	1356	CE2	TYR	228	-2.448	18.587	14.265	1.00	30.74
MOTA	1357	CZ	TYR	228	-1.344	19.196	14.838	1.00	32.92
ATOM	1358	ОН	TYR	228	-1.366	20.546	15.102	1.00	39.97
MOTA	1359	C	TYR	228	-2.260	12.829	13.438	1.00	24.23
ATOM	1360	0	TYR	228	-1.750	12.451	12.379	1.00	25.15
ATOM	1361	N	TYR	229	-2.525	12.000	14.449	1.00	23.04
MOTA	1362	CA	TYR	229	-2.204	10.575	14.355	1.00	17.62
MOTA	1363	CB	TYR	229	-1.270	10.177	15.503	1.00	15.95 7.25
MOTA	1364	CG	TYR	229	0.000	10.991	15.552	1.00	7.25
MOTA	1365	CD1	TYR	229	-0.005	12.295	16.034	1.00	
ATOM	1366	CE1	TYR	229	1.151	13.057	16.045	1.00	2.00
MOTA	1367	CD2	TYR	229	1.204	10.472	15.092	1.00	2.00
MOTA	1368	CE2	TYR	229	2.367	11.234	15.101	1.00	2.00
ATOM	1369	CZ	TYR	229	2.326	12.520	15.580	1.00	3.35 7.73
MOTA	1370	OH	TYR	229	3.451	13.286	15.593	1.00	17.31
ATOM	1371	C	TYR .	229	-3.410	9.647	14.305	1.00	14.75
MOTA	1372	0	TYR	229	-3.267	8.427	14.212	1.00	19.16
MOTA	1373	N	ARG	230	-4.602	10.226	14.314	1.00	23.52
MOTA	1374	CA	ARG	230	-5.818	9.426	14.268	1.00 1.00	23.61
MOTA	1375	CB	ARG	230	-6.995	10.208	14.865		28.96
MOTA	1376	CG	ARG	230	-6.688	10.667	16.293	1.00 1.00	30.92
MOTA	1377	CD	ARG	230	-7.900	11.083	17.092	1.00	34.96
MOTA	1378	NE	ARG	230	-7.468	11.590	18.395	1.00	36.46
MOTA	1379	CZ	ARG	230	-8.274	11.863	19.418 19.319	1.00	37.33
MOTA	1380		ARG	230	-9.585	11.685		1.00	35.13
ATOM	1381	NH2		230	-7.760	12.341	20.544	1.00	26.24
MOTA	1382	C	ARG	230	-6.117	8.922	12.849 11.850	1.00	29.78
MOTA	1383	0	ARG	230	-5.851	9.605	12.788	1.00	22.73
MOTA	. 1384	N	ALA	231	-6.648	7.706	11.531	1.00	18.49
MOTA	1385	CA	ALA	231	-6.968	7.037	11.755		15.82
MOTA	1386	CB	ALA	231	-7.110	5.543	10.886	1.00	16.95
MOTA	1387	С	ALA	231	-8.230	7.596	11.567	1.00	19.43
MOTA	1388	0	ALA	231	-9.102	8.128	9.556	1.00	13.15
MOTA	1389	N	PRO	232	-8.352	7.458 6.952	8.668	1.00	10.64
MOTA	1390	CD	PRO	232	-7.287		8.767	1.00	8.39
MOTA	1391	CA	PRO	232	-9.488	7.930	7.373	1.00	9.88
MOTA	1392	CB	PRO	232	-9.153	7.395 7.536	7.325	1.00	6.53
MOTA	1393	CG	PRO	232	-7.654	7.336	9.254	1.00	9.91
ATOM	1394	C	PRO	232	-10.852		9.229	1.00	4.70
MOTA	1395	0	PRO	232	-11.823	8.220 6.223	9.744	1.00	16.52
MOTA	1396	N	GLU	233	-10.908	5.636	10.238	1.00	17.87
MOTA	1397	CA	GLU	233	-12.157	4.097	10.238	1.00	17.61
MOTA	1398	CB	GLU	233	-12.083	3.502	11.228	1.00	24.07
MOTA	1399	CG	GLU	233	-11.054	3.091	10.545	1.00	23.95
MOTA	1400	CD	GLU	233	-9.764	3.891	9.762	1.00	32.58
ATOM	1401		LGLU	233	-9.227	1.964	10.787	1.00	20.43
MOTA	1402		2 GLU	233	-9.283	6.193	11.593	1.00	21.23
MOTA	1403	C	GLU	233	-12.584 -13.756	6.081		1.00	22.33
ATOM	1404		GLU	233	-13.756	6.786		1.00	19.53
MOTA	1405		VAL	234	-11.920	7.393		1.00	16.80
MOTA	1406			234	-10.672	7.385		1.00	15.57
MOTA	1407			234		8.082		1.00	20.84
MOTA	1408		1 VAL	234	-10.978 -10.235	5.956		1.00	17.05
MOTA	1409		2 VAL		-10.235	8.837		1.00	19.12
MOTA	1410		VAL	234	-12.336			1.00	21.96
MOTA	1411		VAL	234	-13.415			1.00	19.93
MOTA	1412		ILE	235	-11.889				14.90
MOTA	1413			235	-11.859				6.48
MOTA	1414	CB	ILE	235	-10.030	,			

# FIG. 1Y

MOTA	1415	CG2	ILE	235	-11.216	12.918	10.742	1.00	11.04
MOTA	1416	CG1	ILE	235	-9.439	11.479	11.682	1.00	3.71 2.00
ATOM	1417	CD1	ILE	235	-8.390	11.912	10.670	1.00	16.32
MOTA	1418	C	ILE	235	-13.255	11.029	11.447	1.00	21.85
MOTA	1419	Ο,	ILE	235	-13.968	12.015	11.618	1.00	20.37
MOTA	1420	N	LEU	236	-13.600	10.021	10.647	1.00 1.00	21.61
MOTA	1421	CA	LEU	236	-14.871	10.025	9.921		17.45
ATOM	1422	CB	LEU	236	-14.652	9.597	8.469	1.00	21.12
MOTA	1423	CG	LEU	236	-13.731	10.515	7.653 6.275	1.00 1.00	19.91
MOTA	1424	CD1		236	-13.497	9.937		1.00	17.10
MOTA	1425	CD2		236	-14.315	11.913	7.533	1.00	23.24
MOTA	1426	C	LEU	236	-15.990	9.212	10.566	1.00	23.76
MOŢA	1427	0	LEU	236	-17.148	9.325	10.175	1.00	29.40
MOTA	1428	N	GLY	237	-15.638	8.410	11.567	1.00	29.75
MOTA	1429	CA	GLY	237	-16.611	7.597	12.277	1.00	31.11
MOTA	1430	С	GLY	237	-17.297	6.528	11.457 11.220	1.00	31.67
MOTA	1431	0	GLY	237	-18.505	6.598	11.220	1.00	33.24
MOTA	1432	N	MET	238	-16.530	5.528	10.232	1.00	40.35
MOTA	1433	CA	MET	238	-17.072	4.430	8.911	1.00	42.67
MOTA	1434	CB	MET	238	-16.294	4.322	8.015	1.00	43.24
MOTA	1435	CG	MET	238	-16.364	5.541	6.744	1.00	45.00
MOTA	1436	SD	MET	238	-15.094	5.451	7.497	1.00	45.15
MOTA	1437	CE	MET	238	-13.860	6.403	10.958	1.00	38.94
MOTA	1438	С	MET	238	-16.997	3.081	10.410	1.00	41.45
MOTA	1439	0	MET	238	-17.393	2.045	12.203	1.00	35.34
MOTA	1440	N	GLY	239	-16.535	3.098	12.205	1.00	32.28
MOTA	1441	CA	GLY	239	-16.375	1.855 1.531	12.758	1.00	28.98
MOTA	1442	C	GLY	239	-14.904	2.181	11.949	1.00	31.47
MOTA	1443	0	GLY	239	-14.227	0.518	13.454	1.00	23.63
MOTA	1444	N	TYR	240	-14.400	0.208	13.356	1.00	14.17
MOTA	1445	CA	TYR	240	-12.976	1.131	14.309	1.00	20.41
MOTA	1446	CB	TYR	240	-12.192	1.072	15.757	1.00	23.03
MOTA	1447	CG	TYR	240	-12.658 -11.957	0.341	16.711	1.00	18.92
MOTA	1448		TYR	240	-12.412	0.252	18.031	1.00	18.94
MOTA	1449	CE1		240	-13.826	1.720	16.165	1.00	22.91
MOTA	1450	CD2		240	-14.282	1.633	17.484	1.00	23.42
ATOM	1451	CE2		240	-13.573	0.896	18.405	1.00	23.41
MOTA	1452	CZ	TYR	240	-14.041	0.786	19.693	1.00	31.32
MOTA	1453	OH	TYR	240 240	-12.668	-1.236	13.699	1.00	12.19
MOTA	1454	C	TYR		-13.571	-2.027	14.019	1.00	10.14
MOTA	1455	0	TYR	240 241	-11.384	-1.572	13.613	1.00	3.54
MOTA	1456	N	LYS	241	-10.892	-2.896	13.956	1.00	6.13
MOTA	1457	CA		241	-11.100	-3.908	12.811	1.00	8.75
ATOM	1458	CB	LYS	241	-10.067		11.690	1.00	10.54
ATOM	1459	CG	LYS	241	-10.537		10.543	1.00	11.62
ATOM	1460	CD	LYS	241	-9.530		9.401	1.00	11.38
ATOM	1461	CE	LYS	241	-10.032		8.231	1.00	21.31
ATOM	1462	NZ	LYS	241	-9.430		14.368	1.00	5.59
MOTA	1463	C	LYS	241	-8.872	_	14.342	1.00	6.19
MOTA	1464	0	LYS	241	-8.804		14.739	1.00	9.26
MOTA	1465	N	GLU		-7.423		15.198	1.00	12.44
MOTA	1466	CA	GLU	242	-6.847		15.424	1.00	11.72
ATOM	1467	CB	GLU	242	-7.788		15.179	1.00	17.26
ATOM	1468	CG	GLU	242	-8.706			1.00	13.46
ATOM	1469	CD	GLU	242	-8.191			1.00	20.43
MOTA	1470		1 GLU	242	-9.937			1.00	15.86
MOTA	1471		2 GLU	242	-6.444			1.00	14.72
MOTA	1472		GLU	242	-5.565			1.00	21.41
MOTA	1473	0	GLU	242	, 5.505				



#### FIG. 1Z

ATOM	1474	N	ASN	243	-6.587	-3.013	13.050		19.31
ATOM	1475	CA	ASN	243	-5.613	-2.277	12.248	1.00	21.03
ATOM	1476	CB	ASN	243	-5.559	-2.800	10.799	1.00	21.90
MOTA	1477	CG	ASN	243	-6.795	-2.463	9.992	1.00	22.02
ATOM	1478	OD1	ASN	243	-7.752	-1.884	10.502	1.00	25.24
MOTA	1479	ND2	ASN	243	-6.770	-2.811	8.713	1.00	26.83
ATOM	1480	C	ASN	243	-5.729	-0.752	12.318	1.00	19.59
MOTA	1481	0	ASN	243	-4.985	-0.033	11.651	1.00	21.35
ATOM	1482	N	VAL	244	-6.609	-0.254	13.180	1.00	16.86
MOTA	1483	CA	VAL	244.	-6.764	1.183	13.322	1.00	12.16 6.16
ATOM	1484	CB	VAL	244	-8.023	1.555	14.132	1.00	5.57
ATOM	1485	CG1	VAL	244	-7.913	1.067	15.554	1.00	3.91
MOTA	1486	CG2	VAL	244	-8.271	3.048	14.067	1.00	12.08
MOTA	1487	C	VAL	244	-5.517	1.766	13.967	1.00	17.02
MOTA	1488	0	VAL	244	-5.170	2.921	13.738	1.00	10.69
MOTA	1489	N	ASP	245	-4.800	0.934	14.714	1.00	7.76
MOTA	1490	CA	ASP	245	-3.578	1.372	15.378	1.00	14.73
MOTA	1491	CB	ASP	245	-3.309	0.543	16.641	1.00	15.38
ATOM	1492	CG	ASP	245	-4.325	0.794	17.735	1.00	
ATOM	1493	OD1	ASP	245	-4.728	1.967	17.889	1.00	14.39
MOTA	1494	OD2	ASP	245	-4.720	-0.170	18.426	1.00	9.85
ATOM	1495	C	ASP	245	-2.399	1.252	14.460	1.00	5.82
MOTA	1496	0	ASP	245	-1.287	1.611	14.832	1.00	8.10
MOTA	1497	N	ILE	246	-2.611	0.662	13.291	1.00	11.60
ATOM	1498	CA	ILE	246	-1.529	0.509	12.318	1.00	14.99
MOTA	1499	CB	ILE	246	-1.806	-0.674	11.316	1.00	15.80
ATOM	1500	CG2	ILE	246	-0.951	-0.557	10.049	1.00	17.53
ATOM	1501	CG1	ILE	246	-1.498	-2.014	11.999	1.00	9.33
ATOM	1502	CD1	ILE	246	-0.022	-2.248	12.261	1.00	2.50
ATOM	1503	C	ILE	246	-1.310	1.847	11.599	1.00	11.65
ATOM	1504	0	ILE	246	-0.174	2.223	11.300	1.00	12.98
ATOM	1505	N	TRP	247	-2.390	2.607	11.422	1.00	13.04
ATOM	1506	CA	TRP	247	-2.305	3.913	10.784	1.00	13.02
ATOM	1507	CB	TRP	247	-3.670	4.593	10.747.		15.24
ATOM	1508	ĊĠ	TRP	247	-3.591	6.016	10.254	1.00	25.04
ATOM	1509	CD2	TRP	247	-3.678	6.466	8.891	1.00	29.15
ATOM	1510	CE2		247	-3.507	7.868	8.903	1.00	32.78
ATOM	1511	CE3		247	-3.872	5.820	7.666	1.00	27.68
ATOM	1512	CD1		247	-3.382	7.144	11.010	1.00	24.32
ATOM	1513	NE1		247	-3.332	8.254	10.209	1.00	22.09
ATOM	1514	CZ2		247	-3.527	8.635	7.723	1.00	33.21
ATOM	1515	CZ3		247	-3.894	6.578	6.504	1.00	23.18
ATOM	1516	CH		247	-3.721	7.967	6.538	1.00	27.77
ATOM	1517		TRP	247	-1.345	4.789	11.577	1.00	15.01
ATOM	1518		TRP	247	-0.313	5.238	11.065	1.00	16.99
MOTA	1519		SER	248	-1.662	4.948	12.860	1.00	14.45
MOTA	1520		SER	248	-0.891	5.771	13.784	1.00	12.48
ATOM	1521		SER	248	-1.533	5.716	15.168	1.00	13.86
ATOM	1522			248	-2.952	5.797	15.062	1.00	13.99
ATOM	1523		SER	248	0.580	5.370	13.850	1.00	11.77
ATOM	1524		SER	248	1.449	6.225	14.042	1.00	16.52
ATOM	1525		VAL	249	0.865		13.681	1.00	11.99
ATOM	1525			249	2.247		13.698		8.92
	1526			249	2.304			1.00	
MOTA MOTA	1527		1 VAL		3.735				
ATOM	1529		2 VAL		1.674				10.49
	1529		Z VAL		2.901				
MOTA MOTA	1531		VAL		4.125			1.00	
	1531		GLY		2.065				6.91
MOTA	1004	. 1/1	GLI	230					



#### FIG. 1AA

								1 00	E 25
MOTA	1533	CA	GLY	250	2.548	4.527	10.047	1.00	5.35 4.31
MOTA	1534	C	GLY	250	2.963	5.977	10.119 9.724	1.00	4.22
MOTA	1535	0	GLY	250	4.077	6.338	10.678	1.00	7.44
MOTA	1536	N	CYS	251	2.076	6.799	10.856	1.00	2.00
MOTA	1537	CA	CYS	251	2.312	8.230	11.601	1.00	2.00
MOTA	1538	CB	CYS	251	1.138	8.858	10.799	1.00	2.78
MOTA	1539	SG	CYS	251	-0.474	8.661	11.631	1.00	6.97
MOTA	1540	C	CYS	251	3.616	8.467	11.031		12.60
ATOM	1541	0	CYS	251	4.438	9.292	12.709	1.00	7.61
MOTA	1542	N	ILE	252	3.823	7.706	13.556	1.00	6.09
MOTA	1543	CA	ILE	252	5.019	7.810	14.831	1.00	4.83
MOTA	1544	CB	ILE	252	4.871	6.950 6.808	15.530	1.00	2.00
MOTA	1545	CG2	ILE	252	6.218	7.533	15.739	1.00	9.15
MOTA	1546	CG1	ILE	252	3.785	6.618	16.876	1.00	8.65
MOTA	1547	CD1	ILE	252	3.368	7.349	12.827	1.00	6.13
MOTA	1548	С	ILE	252	6.274	7.934	12.981	1.00	8.25
MOTA	1549	0	ILE	252	7.345	6.255	12.083	1.00	12.21
MOTA	1550	N	MET	253	6.147	5.700	11.321	1.00	9.31
MOTA	1551	CA	MET	253	7.260	4.378	10.689	1.00	12.07
MOTA	1552	CB	MET	253	6.843 7.951	3.710	9.911	1.00	17.77
MOTA	1553	CG	MET	253	7.378	2.346	8.895	1.00	14.25
ATOM	1554	SD	MET	253	8.981	1.704	8.404	1.00	2.00
MOTA	1555	CE	MET	253	7.670	6.688	10.230	1.00	6.53
MOTA	1556	C	MET	253	8.856	6.991	10.063	1.00	6.83
MOTA	1557	0	MET	253	6.674	7.231	9.530	1.00	7.59
MOTA	1558	N	GLY	254	6.927	8.196	8.473	1.00	14.92
MOTA	1559	CA	GLY	254	7.597	9.453	9.010	1.00	19.52
MOTA	1560	C	GLY	254	8.446	10.057	8.346	1.00	22.42
MOTA	1561	0	GLY	254 255	7.242	9.813	10.240	1.00	15.34
MOTA	1562	N	GLU	255 255	7.779	10.975	10.924	1.00	8.43
MOTA	1563	CA	GLU	255	6.897	11.265	12.124	1.00	10.24
MOTA	1564	CB	GLU	255	7.168	12.568	12.834	1.00	6.53
MOTA	1565	CG	GLU	255	6.188	12.798	13.961	1.00	8.13
MOTA	1566	CD OE:		255	4.984	12.542	13.770	1.00	11.86
MOTA	1567	OE:		255	6.616	13.241	15.034	1.00	16.77
ATOM	1568	C C	GLU	255	9.219	10.734	11.369	1.00	6.94
MOTA	1569	0	GTA	255	10.010	11.670	11.503	1.00	7.55
MOTA	1570	И	MET	256	9.575	9.475	11.584	1.00	10.29
MOTA	1571			256	10.926	9.155	12.008	1.00	14.75
MOTA	1572	CB	MET	256	11.005	7.723	12.561	1.00	15.70
ATOM	1573 1574			256	10.308	7.560	13.918	1.00	17.40
MOTA	1575			256	10.091	5.868	14.551	1.00	20.23
MOTA	1576			256	11.669	5.57 <b>7</b>	15.143	1.00	5.04
MOTA	1577		MET	256	11.889	9.368	10.854	1.00	13.20
MOTA		_	MET	256	13.065	9.670	11.069	1.00	15.06
MOTA	1578 1579		VAL	257	11.383	9.226	9.630		18.22
MOTA	1579			257	12.204	9.418	8.436	1.00	17.33
MOTA	1581			257	11.888	8.413	7.292		10.85
MOTA	1582		1 VAL	257	12.854	7.265			16.21
ATOM	1582		2 VAL	257	10.486	7.908	7.389	1.00	7.85
MOTA	1584		VAL	257	12.095	10.834	7.884	1.00	18.77
MOTA	1585		VAL	257	13.087	11.405	7.432	1.00	22.01
MOTA	1586		ARG		10.902	11.414	1.950		
ATOM	1587				10.687	12.76			_
MOTA	1588				9.202	12.972			_
MOTA	1589				8.928	14.159			
MOTA MOTA	1503				7.457	14.274			_
MOTA	159				7.054	13.46	4.727	7 1.00	28.26
MION	100.		110						



# FIG. 1BB

ATOM	1592	CZ	ARG	258	5.796	13.362	4.296	1.00	26.76
MOTA	1593	NH1	ARG	258	4.824	14.004	4.930	1.00	28.87
ATOM	1594	NH2		258	5.509	12.661	3.207	1.00	24.96
ATOM	1595	C	ARG	258	11.173	13.806	8.456	1.00	25.86
ATOM	1596	0	ARG	258	11.658	14.870	8.070	1.00	32.18
MOTA	1597	N	HIS	259	11.109	13.446	9.740	1.00	24.12
MOTA	1598	CA	HIS	259	11.494	14.313	10.857	1.00	22.37
ATOM	1599	CB	$\mathtt{HIS}$	259	12.851	14.986	10.603	1.00	21.43
ATOM	1600	CG	HIS	259	14.019	14.066	10.746	1.00	18.22
ATOM	1601	CD2	HIS	259	15.287	14.145	10.278	1.00	24.02
MOTA	1602	ND1	HIS	259	13.946	12.882	11.446	1.00	16.87
MOTA	1603	CE1	HIS	259	15.114	12.273	11.405	1.00	22.04
MOTA	1604	NE2	$\mathtt{HIS}$	259	15.947	13.017	10.703	1.00	20.47
ATOM	1605	С	HIS	259	10.438	15.366	11.158	1.00	22.70
MOTA	1606	0	HIS	259	10.588	16.154	12.093	1.00	25.27
MOTA	1607	N	LYS	260	9.369	15.367	10.368	1.00	17.40
ATOM	1608	CA	LYS	260	8.294	16.332	10.524	1.00	16.56
ATOM	1609	CB	LYS	260	8.265	17.268	9.312	1.00	19.39
ATOM	1610	CG	LYS	260	9.626	17.663	8.747	1.00	20.30
MOTA	1611	CD	LYS	260	9.443	18.546	7.519	1.00	28.30
MOTA	1612	CE	LYS	260	10.776	18.964	6.903	1.00	31.46
MOTA	1613	NZ	LYS	260	10.589	19.953	5.801	1.00	36.52
MOTA	1614	C	LYS	260	6.952	15.613	10.608	1.00	19.33
MOTA	1615	0	LYS	260	6.770	14.556	10.000	1.00	17.65
MOTA	1616	N	ILE	261	5.996	16.201	11.326	1.00	17.62
ATOM	1617	CA	ILE	261	4.668	15.602	11.449	1.00	14.19
MOTA	1618	CB	ILE	261	3.696	16.442	12.337	1.00	7.20
ATOM	1619	CG2		261	2.279	15.854	12.304	1.00	2.00 10.49
MOTA	1620	CG1		261	4.196	16.473	13.784	1.00	3.19
ATOM	1621	CD1		261	3.166	16.993	14.778	1.00 1.00	15.65
MOTA	1622	C	ILE	261	4.063	15.434	10.061 9.332	1.00	15.94
MOTA	1623	0	ILE	261	3.865	16.401	9.736	1.00	16.99
MOTA	1624	N	LEU	262	3.764	14.183 13.773	8.460	1.00	16.61
MOTA	1625	CA	LEU	262	3.193	12.272	8.519	1.00	14.07
MOTA	1626	CB	LEU	262	2.889 3.555	11.337	7.510	1.00	11.45
ATOM	1627	CG	LEU	262	5.061	11.292	7.728	1.00	7.82
MOTA	1628	CD1		262	2.931	9.958	7.638	1.00	3.94
MOTA	1629	CD2		262	1.930	14.541	8.025	1.00	19.12
MOTA	1630	C	LEU	262	1.886	15.071	6.909	1.00	20.84
MOTA	1631	0	LEU PHE	262 263	0.909	14.571	8.877	1.00	19.61
ATOM	1632	N CA	PHE	263	-0.344	15.263	8.556	1.00	19.23
MOTA	1633 1634	CB	PHE	263	-1.498	14.264	8.419	1.00	20.11
MOTA MOTA	1635	CG	PHE	263	-1.123	12.991	7.714	1.00	31.62
	1636		. PHE	263	-0.890	12.976	6.343	1.00	32.52
ATOM ATOM	1637		PHE	263	-1.007	11.800	8.425	1.00	32.72
ATOM	1638		. PHE	263	-0.536	11.788	5.685	1.00	31.61
MOTA	1639		PHE	263	-0.655	10.606	7.784	1.00	31.76
MOTA	1640	CZ	PHE	263	-0.418	10.600	6.407	1.00	27.52
ATOM	1641	C	PHE	. 263	-0.714	16.277	9.643	1.00	21.98
ATOM	1642	ō	PHE	263	-1.630	16.035	10.434	1.00	24.79
MOTA	1643	И	PRO	264	-0.020	17.428	9.690	1.00	22.78
ATOM	1644	CD	PRO	264	1.169	17.776	8.894	1.00	22.19
ATOM	1645	CA	PRO	264	-0.297	18.467	10.693	1.00	24.13
ATOM	1646	CB	PRO	264	1.035	19.210	10.774	1.00	21.59
ATOM	1647	CG	PRO	264	1.478	19.199	9.349	1.00	23.37
ATOM	1648	C	PRO	264	-1.456	19.396	10.319	1.00	24.33
ATOM	1649	Ö	PRO	264	-1.250	20.502	9.817	1.00	28.26
MOTA	1650	N	GLY		-2.674	18.939	10.587	1.00	23.20
712 OF			~~.	200		•			

# FIG. 1CC

ATOM	1651	CA	GLY	265	-3.860	19.716	10.276	1.00	31.03 37.14
MOTA	1652	C	GLY	265	-4.302	20.680	11.361	1.00	39.17
MOTA	1653	0	GLY	265	-4.579	20.264 21.961	12.488 11.007	1.00	39.70
ATOM	1654	N	ARG	266	-4.404	23.013	11.933	1.00	38.28
MOTA	1655	CA	ARG	266	-4.816	24.374	11.255	1.00	40.99
MOTA	1656	CB	ARG	266	-4.703	24.374	10.975	1.00	47.16
MOTA	1657	CG	ARG	266	-3.263	26.160	10.337	1.00	50.47
MOTA	1658	CD	ARG	266	-3.171	26.100	10.877	1.00	52.30
MOTA	1659	NE	ARG	266	-2.047	26.921	10.461	1.00	54.85
MOTA	1660	CZ	ARG	266	-0.786	25.988	9.476	1.00	54.82
MOTA	1661	NH1		266	-0.462 0.165	27.528	11.061	1.00	55.46
ATOM	1662		ARG	266	-6.212	22.845	12.527	1.00	40.23
ATOM	1663	C	ARG	266	-6.500	23.392	13.594	1.00	42.31
MOTA	1664	0	ARG	266	-7.079	22.113	11.829	1.00	39.95
ATOM	1665	N	ASP	267 267	-8.445	21.866	12.291	1.00	36.79
ATOM	1666	CA	ASP	267 267	-9.381	23.043	11.933	1.00	42.01
ATOM	1667	CB	ASP	267	-9.255	23.504	10.475	1.00	42.09
ATOM	1668	CG	ASP	267	-10.263	23.420	9.734	1.00	37.79
ATOM	1669		ASP	267	-8.171	23.997	10.084	1.00	42.40
ATOM	1670		ASP ASP	267	-8.989	20.531	11.776	1.00	34.35
MOTA	1671	C	ASP	267	-8.265	19.776	11.120	1.00	35.42
ATOM	1672	O N	ALA	268	-10.257	20.245	12.073	1.00	31.62
MOTA	1673	CA	ALA	268	-10.903	18.999	11.659	1.00	30.64
ATOM	1674 1675	CB	ALA	268	-12.337	18.955	12.188	1.00	28.57
MOTA	1675	C	ALA	268	-10.907	18.852	10.138	1.00	32.52
ATOM ATOM	1677	0	ALA	268	-10.762	17.746	9.599	1.00	28.70
ATOM	1678	N	ILE	269	-11.014	19.994	9.460	1.00	33.35
ATOM	1679	CA	ILE	269	-11.055	20.071	8.003	1.00	26.07
ATOM	1680	CB	ILE	269	-11.705	21.398	7.595	1.00	24.01
ATOM	1681	CG2		269	-11.614	21.610	6.087	1.00	24.76
ATOM	1682	CG1		269	-13.149	21.403	8.105	1.00	25.34
ATOM	1683	CD1		269	-13.785	22.763	8.199	1.00	20.60
ATOM	1684	C	ILE	269	-9.682	19.927	7.367	1.00	20.53
MOTA	1685	0	ILE	269	-9.492	19.133	6.459	1.00	20.91
ATOM	1686	N	ASP	270	-8.716	20.659	7.901	1.00	21.56
ATOM	1687	CA	ASP	270	-7.353	20.632	7.398	1.00	20.48
ATOM	1688	CB	ASP	270	-6.531	21.735	8.057	1.00	20.75
ATOM	1689	CG	ASP	270	-5.205	21.970	7.366	1.00	23.84
MOTA	1690	OD1	ASP	270	-5.172	21.986	6.113	1.00	28.48
MOTA	1691	OD2	ASP	270	-4.192	22.162	8.077	1.00	27.78
MOTA	1692	C	ASP	270	-6.685	19.290	7.640	1.00	23.87
MOTA	1693	0	ASP	270	-5.709	18.962	6.971	1.00	22.94
MOTA	1694	N	GLN	271	-7.185	18.524	8.610	1.00	27.87
MOTA	1695	CA	GLN	271	-6.611	17.213	8.917	1.00	26.15 29.33
MOTA	1696	CB	GLN	271	-7.225	16.634	10.200	1.00	30.10
MOTA	1697	CG	GLN	271	-6.560	15.344	10.683	1.00	33.24
MOTA	1698	CD	GLN	271	-5.054	15.469	10.774	1.00	30.97
MOTA	1699	OE	L GLN	271	-4.317	14.813	10.038	1.00	36.55
MOTA	1700	NE		271	-4.588	16.345	11.655	1.00 1.00	23.40
MOTA	1701	С	GLN	271	-6.800	16.227	7.766	1.00	17.83
MOTA	1702	0	GLN	271	-5.843	15.587	7.330	1.00	21.41
MOTA	1703	N	TRP	272	-8.032	16.126	7.270 6.174	1.00	21.41
MOTA	1704	CA	TRP	272	-8.352		5.944	1.00	25.91
MOTA	1705	CB	TRP	272	-9.862		4.855	1.00	34.96
ATOM	1706	CG	TRP	272	-10.320		4.856	1.00	37.63
MOTA	1707	CD:		272	-10.216		3.684	1.00	39.04
MOTA	1708	CE:		272	-10.864			1.00	36.23
MOTA	1709	CE:	3 TRP	272	-9.645	11.02/	٠.١٥٥	2.00	

#### FIG. 1DD

									24 40
ATOM	1710	CD1	TRP	272	-11.001	14.559	3.706	1.00	34.40
MOTA	1711	NE1	TRP	272	-11.333	13.420	3.004	1.00	34.42
ATOM	1712	CZ2	TRP	272	-10.954	10.956	3.373	1.00	38.88
ATOM	1713	CZ3	TRP	272	-9.733	10.504	5.427	1.00	33.36
ATOM	1714	CH2	TRP	272	-10.385	10.063	4.257	1.00	37.17
ATOM	1715	C	TRP	272	-7.647	15.626	4.887	1.00	23.52
MOTA	1716	ō	TRP	272	-7.130	14.774	4.165	1.00	25.26
ATOM	1717	N	ASN	273	-7.576	16.930	4.632	1.00	24.61
	1718	CA	ASN	273	-6.947	17.449	3.424	1.00	20.66
MOTA	1719	CB	ASN	273	-7.186	18.954	3.290	1.00	22.38
MOTA			ASN	273	-8.625	19.285	2.939	1.00	22.57
MOTA	1720	CG		273	-9.275	18.551	2.192	1.00	16.68
MOTA	1721		ASN		-9.135	20.389	3.480	1.00	19.51
MOTA	1722		ASN	273	-5.469	17.158	3.394	1.00	18.46
MOTA	1723	C	ASN	273	-	16.944	2.326	1.00	24.72
MOTA	1724	0	ASN	273	-4.893	17.153	4.565	1.00	17.40
ATOM	1725	N	LYS	274	-4.849			1.00	20.54
MOTA	1726	CA	LYS	274	-3.423	16.863	4.681	1.00	24.00
MOTA	1727	CB	LYS	274	-2.946	17.126	6.117		
MOTA	1728	CG	LYS	274	-2.820	18.606	6.490	1.00	23.91
ATOM	1729	CD	LYS	274	-1.570	19.229	5.890	1.00	31.69
ATOM	1730	CE	LYS	274	-1.429	20.711	6.242	1.00	36.12
ATOM	1731	NZ	LYS	274	-2.396	21.581	5.504	1.00	39.86
ATOM	1732	C	LYS	274	-3.170	15.401	4.301	1.00	19.94
ATOM	1733	0	LYS	274	-2.091	15.056	3.815	1.00	17.57
ATOM	1734	N	VAL	275	-4.188	14.561	4.500	1.00	21.20
ATOM	1735	CA	VAL	275	-4.135	13.129	4.195	1.00	21.22
ATOM	1736	CB	VAL	275	-5.260	12.356	4.947	1.00	27.34
	1737		VAL	275	-5.249	10.863	4.570	1.00	24.55
MOTA			VAL	275	-5.100	12.535	6.450	1.00	21.86
ATOM	1738		VAL	275	-4.246	12.822	2.695	1.00	19.42
ATOM	1739	C			-3.321	12.258	2.105	1.00	19.86
MOTA	1740	0	VAL	275	-5.368	13.195	2.078	1.00	15.37
ATOM	1741	N	ILE	276		12.949	0.655	1.00	10.70
MOTA	1742	CA	ILE	276	-5.561		0.033	1.00	2.68
MOTA	1743	CB	ILE	276	-7.020	13.177	1.052	1.00	2.00
MOTA	1744	CG2		276	-7.948	12.312			2.00
ATOM	1745	CG1		276	-7.393	14.642	0.337	1.00	2.00
MOTA	1746	CD1	ILE	276	-8.879	14.892	0.120	1.00	
MOTA	1747	C	ILE	276	-4.608	13.728	-0.244	1.00	11.53
ATOM	1748	0	ILE	276	-4.358	13.332	-1.378	1.00	13.01
MOTA	1749	N	GLU	277	-4.034	14.810	0.258	1.00	17.68
ATOM	1750	CA	GLU	277	-3.085	15.574	-0.546	1.00	21.93
MOTA	1751	CB	GLU	277	-2.609	16.805	0.228	1.00	26.73
ATOM	1752	CG	GLU	277	-3.333	18.094	-0.107	1.00	31.15
ATOM	1753	CD	GLU	277	-3.082	19.186	0.920	1.00	31.05
ATOM	1754		GLU	277	-1.907	19.418	1.278	1.00	28.67
	1755		GLU	277	-4.066	19.805	1.378	1.00	30.92
ATOM		C	GLU	277	-1.879	14.694	-0.874	1.00	23.55
ATOM	1756			277	-1.367	14.704	-2.002	1.00	25.88
ATOM	1757	0	GLU		-1.471	13.895	0.111	1.00	20.15
MOTA	1758	N	GLN	278	-0.310	13.018	-0.002	1.00	17.85
MOTA	1759	CA	GLN	278		12.945	1.335	1.00	15.48
MOTA	1760	CB	GLN	278	0.412			1.00	13.04
MOTA	1761	CG	GLN	278	0.945		1.858		9.75
MOTA	1762	CD	GLN	278	1.552		3.223	1.00	
MOTA	1763		l GLN	278	2.682		3.359	1.00	9.48
MOTA	1764	NE:	2 GLN	278	0.796		4.246	1.00	12.91
ATOM	1765	C	GLN	278	-0.591		-0.435	1.00	15.71
ATOM	1766		GLN	278	0.260		-1.055	1.00	16.36
ATOM	1767		LEU	279	-1.753		-0.055	1.00	11.53
ATOM	1768			279	-2.115	9.711	-0.367	1.00	12.00

## FIG. 1EE

MOTA	1769	CB	LEU	279	-2.639	9.017	0.887	1.00	12.00
MOTA	1770	CG	LEU	279	-1.786	9.084	2.158	1.00	9.51
MOTA	1771	CD1	LEU	279	-2.339	8.079	3.146	1.00	6.61
MOTA	1772	CD2	LEU	279	-0.315	8.805	1.867	1.00	3.14
MOTA	1773	С	LEU	279	-3.124	9.578	-1.500	1.00	17.06
MOTA	1774	0	LEU	279	-3.161	8.562	-2.198	1.00	18.67
MOTA	1775	N	GLY	280	-3.926	10.613	-1.696	1.00	18.66
ATOM	1776	CA	GLY	280	-4.909	10.587	-2.757	1.00	15.54
ATOM	1777	С	GLY	280	-6.307	10.343	-2.251	1.00	16.01
MOTA	1778	0	GLY	280	-6.505	9.822	-1.153	1.00	18.83
ATOM	1779	N	THR	281	-7.287	10.740	-3.045	1.00	17.90
ATOM	1780	CA	THR	281	-8.676	10.558	-2.678	1.00	20.47
MOTA	1781	CB	THR	281	-9.603	11.349	-3.622	1.00	16.28
MOTA	1782	0G1	THR	28,1	-9.144	12.706	-3.706	1.00	17.45
MOTA	1783	CG2	THR	281	-11.037	11.351	-3.112	1.00	17.34
MOTA	1784	С	THR	281	-8.975	9.062	-2.748	1.00	26.86
MOTA	1785	0	THR	281	-8.603	8.394	-3.712	1.00	31.52
ATOM	1786	N	PRO	282	-9.563	8.511	-1.680	1.00	28.38
MOTA	1787	CD	PRO	282	-9.854	9.208	-0.418	1.00	25.29
MOTA	1788	CA	PRO	282	-9.919	7.092	-1.573	1.00	26.47
MOTA	1789	CB	PRO	282	-10.421	6.980	-0.136	1.00	21.64
ATOM	1790	CG	PRO	282	-10.959	8.351	0.155	1.00	21.02
MOTA	1791	С	PRO	282	-10.960	6.570	-2.560	1.00	25.85
MOTA	1792	0	PRO	282	-11.840	7.299	-3.022	1.00	25.44
MOTA	1793	N	CYS	283	-10.855	5.269	-2.822	1.00	25.32
MOTA	1794	CA	CYS	283	-11.722	4.532	-3.729	1.00	24.18
MOTA	1795	CB	CYS	283	-11.255	3.071	-3.797	1.00	26.45
ATOM	1796	SG	CYS	283	-11.206	2.192	-2.201	1.00	38.53
MOTA	1797	C	CYS	283	-13.171	4.600	-3.285	1.00	20.79
MOTA	1798	0	CYS	283	-13.449	4.791	-2.113	1.00	25.27
ATOM	1799	N	PRO	284	-14.117	4.474	-4.231	1.00	21.61
MOTA	1800	CD	PRO	284	-13.890	4.378	-5.686	1.00	17.56
MOTA	1801	CA	PRO	284	~15.555	4.515	-3.926	1.00	18.26
MOTA	1802	CB	PRO	284	-16.199	4.309	-5.299	1.00	20.65
ATOM	1803	CG	PRO	284	-15.185	4.905	-6.246	1.00	17.52
ATOM	1804	C	PRO	284	-15.974	3.424	-2.943	1.00	19.06
MOTA	1805	0	PRO	284	-17.050	3.483	-2.358	1.00	20.50
MOTA	1806	N	ALA	285	-15.126	2.411	-2.788	1.00	21.71
ATOM	1807	CA	ALA	285	-15.394	1.310	-1.878	1.00	26.28
MOTA	1808	CB	ALA	285	-14.325	0.234	-2.043	1.00	26.44
ATOM	1809	C	ALA	285	-15.393	1.848	-0.446	1.00	27.71
ATOM	1810	0	ALA	285	-16.212	1.451	0.388	1.00	29.33
MOTA	1811	N	PHE	286	-14.462	2.763	-0.193		27.78
MOTA MOTA	1812 1813	CA	PHE	286 286	-14.289 -12.940	3.409 4.118	1.098 1.097	1.00 1.00	23.59 24.13
ATOM	1814	CB CG	PHE	286	-12.628		2.373	1.00	29.65
ATOM	1815		PHE	286	-12.212	4.831 4.123	3.494	1.00	31.45
ATOM	1816		PHE	286 ·	-12.702	6.216	2.439	1.00	31.48
ATOM	1817		PHE	286	-11.874	4.786	4.664	1.00	32.34
ATOM	1818		PHE	286	-12.368	6.891	3.598	1.00	32.31
ATOM	1819	CEZ	PHE	286	-11.949	6.175	4.716	1.00	32.68
ATOM	1820	C	PHE	286	-15.401	4.425	1.284	1.00	22.60
ATOM	1821	Õ	PHE	286	-16.135	4.391	2.270	1.00	25.95
ATOM	1822	N	MET	287	-15.561	5.291	0.288	1.00	19.48
ATOM	1823	CA	MET	287	-16.570	6.332	0.311	1.00	16.74
ATOM	1824	CB	MET	287	-16.580	7.106	-1.017	1.00	18.72
ATOM	1825	CG	MET	287	-15.314	7.938	-1.283	1.00	20.14
MOTA	1826	SD	MET	287	-14.974	9.280	-0.078	1.00	20.20
MOTA	1827	CE	MET	287	-13.753	10.219	-0.961	1.00	24.44
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#### FIG. 1FF

ATOM	1828	С	MET	287	-17.955	5.782	0.625	1.00	16.03
ATOM	1829	0	MET	287	-18.659	6.331	1.456	1.00	18.99
MOTA	1830	N	ALA	288	-18.317	4.662	0.013	1.00	20.90
ATOM	1831	CA	ALA	288	-19.626	4.066	0.236	1.00	26.22
ATOM	1832	CB	ALA	288	-19.826	2.875	-0.694	1.00	26.60
MOTA	1833	C	ALA	288	-19.833	3.653	1.693	1.00	28.97
ATOM	1834	Ō	ALA	288	-20.966	3.584	2.165	1.00	31.30
ATOM	1835	N	LYS	289	-18.742	3.380	2.407	1.00	32.21
ATOM	1836	CA	LYS	289	-18.829	2.993	3.815	1.00	33.61
ATOM	1837	CB	LYS	289	-17.500	2.391	4.301	1.00	34.28
ATOM	1838	CG	LYS	289	-17.428	0.858	4.209	1.00	34.62
ATOM	1839	CD	LYS	289	-18.440	0.200	5.149	1.00	37.66
ATOM	1840	CE	LYS	289	-18.111	0.495	6.622	1.00	37.54
	1841	NZ	LYS	289	-19.268	0.291	7.549	1.00	34.87
ATOM		C	LYS	289	-19.230	4.193	4.676	1.00	33.97
ATOM	1842			289	-19.769	4.039	5.775	1.00	33.49
MOTA	1843	0	LYS LEU	290	-18.988	5.388	4.147	1.00	35.80
MOTA	1844	N		290	-19.327	6.637	4.827	1.00	35.58
MOTA	1845	CA	LEU		-18.652	7.820	4.134	1.00	31.46
MOTA	1846	CB	LEU	290		7.854	4.011	1.00	30.05
ATOM	1847	CG	LEU	290	-17.135	8.881	2.970	1.00	29.96
MOTA	1848		LEU	290	-16.721	8.166	5.353	1.00	34.22
MOTA	1849		LEU	290	-16.530		4.759	1.00	37.04
MOTA	1850	C	LEU	290	-20.831	6.874	3.719	1.00	39.41
ATOM	1851	0	LEU	290	-21.452	6.666			40.14
MOTA	1852	N .	GLN	291	-21.423	7.317	5.862	1.00	41.39
MOTA	1853	CA	GLN	291	-22.846	7.610	5.849	1.00	
MOTA	1854	CB	GLN	291	-23.442	7.657	7.268	1.00	42.50
ATOM	1855	CG	GLN	291	-22.524	8.174	8.362	1.00	45.42
MOTA	1856	CD	GLN	291	-22.640	7.367	9.650	1.00	48.95
MOTA	1857		GLN	291	-21.630	7.009	10.265	1.00	48.41
MOTA	1858	NE2	GLN	291	-23.871	7.039	10.042	1.00	46.58
ATOM	1859	C	GLN	291	-23.028	8.927	5.091	1.00	41.36
MOTA	1860	0	GLN	291	-22.238	9.856	5.243	1.00	37.77
ATOM	1861	N	PRO	292	-24.047	8.990	4.221	1.00	42.77
MOTA	1862	CD	PRO	292	-25.090	7.948	4.215	1.00	43.22
ATOM	1863	CA	PRO	292	-24.454	10.101	3.360	1.00	40.98
MOTA	1864	CB	PRO	292	-25.969	10.063	3.500	1.00	42.32
MOTA	1865	CG	PRO	292	-26.226	8.589	3.401	1.00	41.51
MOTA	1866	С	PRO	292	-23.866	11.475	3.662	1.00	38.85
MOTA	1867	0	PRO	292	-23.138	12.025	2.835	1.00	37.72
MOTA	1868	N	THR	293	-24.146	11.998	4.853	1.00	36.06
MOTA	1869	CA	THR	293	-23.667	13.319	5.263	1.00	30.91
ATOM	1870	CB	THR	293	-24.095	13.640	6.709	1.00	35.11
ATOM	1871	OG1	THR	293	-25.513	13.472	6.841	1.00	37.56
ATOM	1872		THR	293	-23.701	15.076	7.083	1.00	37.03
ATOM	1873	С	THR	293	-22.151	13.401	5.207	1.00	27.49
ATOM	1874	0	THR	293	-21.587	14.384	4.727	1.00	27.10
ATOM	1875	N			-21.496	12.382	5.749	1.00	26.19
MOTA	1876	CA	VAL	294	-20.046	12.320	5.770	1.00	23.72
ATOM	1877	CB	VAL	294	-19.549	11.159	6.675	1.00	19.37
ATOM	1878		VAL	294	-18.045	11.238	6.874	1.00	13.70
ATOM	1879		VAL	294	-20.263	11.189	8.010	1.00	15.03
ATOM	1880	C	VAL	294	-19.553	12.099	4.345	1.00	29.48
ATOM	1881	Ö	VAL	294	-18.493	12.609	3.955	1.00	33.31
MOTA	1882	N	ARG	295	-20.336	11.368	3.554	1.00	31.18
ATOM	1883	CA	ARG	295	-19.958	11.104	2.169	1.00	30.61
ATOM	1884	CB	ARG	295	-20.976	10.186	1.480	1.00	32.61
ATOM	1885	CG	ARG	295	-20.355	9.204	0.472	1.00	33.15
ATOM	1886	CD	ARG	295	-21.376	8.819	-0.609	1.00	41.22
FIT OU	1000	CD	D/A	275				-	



ATOM	1887	NE	ARG	295	-21.116	7.549	-1.303	1.00	44.77
MOTA	1888	CZ	ARG	295	-20.157	7.332	-2.206	1.00	45.75
MOTA	1889	NH1	ARG	295	-19.314	8.289	-2.560	1.00	42.66
ATOM	1890	NH2	ARG	295	-20.077	6.153	-2.808	1.00	50.09
MOTA	1891	C	ARG	295	-19.893	12.458	1.461	1.00	26.05
ATOM	1892	0	ARG	295	-18.879	12.794	0.855	1.00	27.82
MOTA	1893	N	ASN	296	-20.929	13.272	1.655	1.00	25.63
ATOM	1894	CA	ASN	296	-21.011	14.600	1.048	1.00	23.53
ATOM	1895	CB	ASN	296	-22.313	15.305	1.446	1.00	24.22
MOTA	1896	CG	ASN	296	-23.551	14.648	0.858	1.00	28.67
MOTA	1897	OD1	ASN	296	-23.496	13.529	0.347	1.00	36.26
MOTA	1898	ND2	ASN ·	296	-24.684	15.345	0.928	1.00	30.43
ATOM	1899	С	ASN	296	-19.829	15.470	1.456	1.00	24.99
ATOM	1900	0	ASN	296	-19.059	15.913	0.605	1.00	26.73
MOTA	1901	N	TYR	297	-19.655	15.661	2.762	1.00	26.38
MOTA	1902	CA	TYR	297	-18.582	16.488	3.311	1.00	26.13
MOTA	1903	CB	TYR	297	-18.594	16.387	4.847	1.00	32.32
ATOM	1904	CG	TYR	297	-17.278	16.685	5.538	1.00	32.85
MOTA	1905	CD1	TYR	297	-16.755	17.972	5.580	1.00	32.13
MOTA	1906	CE1	TYR	297	-15.533	18.229	6.202	1.00	34.78
MOTA	1907	CD2	TYR	297	-16.549	15.666	6.139	1.00	34.34
ATOM	1908	CE2	TYR	297	-15.331	15.917	6.758	1.00	36.24
ATOM	1909	CZ	TYR	297	-14.829	17.194	6.785	1.00	34.88
MOTA	1910	OH	TYR	297	-13.613	17.422	7.386	1.00	40.94
ATOM	1911	C	TYR	297	-17.198	16.169	2.746	1.00	23.94
MOTA	1912	0	TYR	297	-16.405	17.077	2.484	1.00	16.61
ATOM	1913	N	VAL	298	-16.936	14.879	2.547	1.00	26.14
ATOM	1914 "	$^{\rm CA}$	VAL	298	-15.665	14.381	2.026	1.00	24.39
MOTA	1915	CB	VAL	298	-15.394	12.936	2.541	1.00	22.80
MOTA	1916		VAL	298	-14.102	12.362	1.941	1.00	19.07
MOTA	1917		VAL	298	-15.302	12.942	4.054	1.00	19.85
ATOM	1918	C	VAL	298	-15.573	14.411	0.497	1.00	25.08
MOTA	1919	0	VAL	298	-14.478	14.520	-0.065	1.00	26.44
ATOM	1920	N	GLU	299	-16.713	14.330	-0.179	1.00	27.22
MOTA	1921	CA	GLU	299	-16.727	14.360	-1.635	1.00	27.74
ATOM	1922	CB	GLU	299	-18.052	13.849	-2.170	1.00	28.52
MOTA	1923	CG	GLU	299	-17.887	12.975	-3.380	1.00	33.99
MOTA	1924	CD	GLU	299	-17.578	11.548	-3.000	1.00	28.84
MOTA	1925		GLU	299	-18.536	10.810	-2.703	1.00	21.31
MOTA	1926	OE2	GLU	299	-16.391	11.164	-2.994	1.00	26.35
MOTA	1927	C	GLU	299	-16.509	15.775	-2.155	1.00	26.19
MOTA	1928	0	GLU	299	-15.767	15.974	-3.113	1.00	27.10
MOTA	1929	N	ASN	300	-17.175	16.749	-1.534	1.00	24.87
MOTA	1930	CA	ASN	300	-17.063	18.148	-1.937	1.00	20.43
MOTA	1931	CB	ASN	300	-18.163	18.979	-1.273	1.00	20.76
MOTA	1932	CG	ASN	300	-18.468	20.260	-2.031	1.00	25.51
MOTA	1933		ASN	300	-17.629	20.784	-2.765	1.00	29.81
MOTA	1934		ASN	300	-19.684	20.768	-1.863	1.00	29.41
MOTA	1935	C	ASN	300	-15.692	18.645	-1.509	1.00	17.56
ATOM	1936	0	ASN	300	-15.553	19.325	-0.500	1.00	21.18
MOTA	1937	N	ARG	301	-14.684	18.282	-2.287	1.00	18.56
MOTA	1938	CA	ARG	301	-13.296	18.637	-2.022	1.00	20.80
ATOM	1939	CB	ARG	301	-12.733	17.754	-0.902	1.00	27.14
MOTA	1940	CG	ARG	301	-12.739	18.365	0.486	1.00	31.25
ATOM	1941	CD	ARG	301	-12.089	17.398	1.454	1.00	30.07
MOTA	1942	NE	ARG	301	-11.876	17.989	2.766	1.00	35.05
MOTA	1943	CZ	ARG	301	-12.796	18.034	3.721	1.00	39.13
MOTA	1944		ARG	301	-14.000	17.516 18.601	3.513 4.888	1.00	34.08
ATOM	1945	MHZ	ARG	301	-12.507	TO . OOT	3.055	1.00	42.53

# FIG. 1HH

	2046	<b>а</b>	NDC!	301	-12.518	18.332	-3.287	1.00	20.56
MOTA	1946	C	ARG ARG	301	-12.956	17.539	-4.101	1.00	23.26
MOTA	1947	N O	PRO	302	-11.349	18.948	-3.464	1.00	21.89
MOTA	1948	CD	PRO	302	-10.670	19.941	-2.619	1.00	25.17
MOTA	1949 1950	CA	PRO	302	-10.572	18.668	-4.670	1.00	25.44
ATOM	1951	CB	PRO	302	-9.407	19.651	-4.559	1.00	26.64
MOTA	1951	CG	PRO	302	-9.236	19.813	-3.084	1.00	24.33
MOTA MOTA	1953	C	PRO	302	-10.086	17.228	-4.661	1.00	29.44
ATOM	1954	0	PRO	302	-9.595	16.750	-3.637	1.00	34.61
ATOM	1955	N	LYS	303	-10.274	16.531	-5.784	1.00	28.85
ATOM	1956	CA	LYS	303	-9.857	15.145	-5.927	1.00	21.63
ATOM	1957	CB	LYS	303	-10.662	14.449	-7.034	1.00	24.46
ATOM	1958	CG	LYS	303	-10.849	15.266	-8.323	1.00	41.84
ATOM	1959	CD	LYS	303	-11.871	14.622	-9.290	1.00	44.46
ATOM	1960	CE	LYS	303	-12.064	15.458	-10.568	1.00	45.69
ATOM	1961	NZ	LYS	303	-13.119	14.930	-11.491	1.00	45.06
ATOM	1962	C	LYS	303	-8.358	15.096	-6.189	1.00	20.81
ATOM	1963	0	LYS	303	-7.807	15.966	-6.858	1.00	20.42
ATOM	1964	N	TYR	304	-7.685	14.130	-5.571	1.00	21.39
ATOM	1965	CA	TYR	304	-6.240	13.971	-5.710	1.00	21.82
ATOM	1966	CB	TYR	304	-5.534	14.211	-4.368	1.00	24.87
ATOM	1967	CG	TYR	304	-5.666	15.594	-3.807	1.00	23.11
ATOM	1968	CD1	TYR	304	-6.777	15.959	-3.050	1.00	23.67
ATOM	1969	CE1	TYR	304	-6.900	17.244	-2.517	1.00	20.86
ATOM	1970	CD2	TYR	304	-4.677	16.545	-4.017	1.00	26.39
MOTA	1971	CE2	TYR	304	-4.795	17.833	-3.486	1.00	24.30
MOTA	1972	$\mathbf{cz}$	TYR	304	-5.907	18.171	-2.742	1.00	23.26
ATOM	1973	OH	TYR	304	-6.032	19.447	-2.251	1.00	28.31
ATOM	1974	C	TYR	304	-5.891	12.563	-6.151	1.00	21.83 21.88
MOTA	1975	0	TYR	304	-6:662	11.623	-5.959	1.00	23.94
MOTA	1976	N	ALA	305	-4.714	12.429	-6.750	1.00	27.30
MOTA	1977	CA	ALA	305	-4.221	11.128	-7.189	1.00	22.41
MOTA	1978	CB	ALA	305	-3.483	11.259	-8.516	1.00 1.00	25.62
MOTA	1979	C	ALA	305	-3.270	10.651	-6.106	1.00	28.28
MOTA	1980	0	ALA	305	-3.089	9.455	-5.893	1.00	23.97
MOTA	1981	N	GLY	306	-2.641	11.617	-5.441	1.00	21.65
MOTA	1982	CA	$\mathbf{G}\mathbf{L}\mathbf{Y}$	306	-1.714	11.321	-4.366	1.00	19.70
MOTA	1983	С	GLY	306	-0.381	10.870	-4.891 -5.837	1.00	21.53
ATOM	1984	0	GLY	306	-0.316	10.093	-4.266	1.00	18.69
MOTA	1985	N	LEU	307	0.686		-4.688	1.00	18.55
MOTA	1986	CA	LEU	307	2.036		-3.984	1.00	15.42
MOTA	1987	CB	LEU	307	3.071		-3.740	1.00	15.82
MOTA	1988	CG	LEU	307	2.718 3.925		-3.745	1.00	9.35
MOTA	1989		LEU	307	2.258		-5.034	1.00	20.09
ATOM	1990		2 LEU	307	2.236			1.00	22.25
MOTA	1991	C	LEU	307	1.692			1.00	27.73
MOTA	1992	0	LEU	307	3.328			1.00	24.37
ATOM	1993	N	THR	308 308	3.758			1.00	23.85
ATOM	1994	CA	THR	308	4.552			1.00	26.19
ATOM	1995	CB	THR	308	5.662		_	1.00	25.39
MOTA	1996		1 THR 2 THR	308	3.654			1.00	26.29
ATOM	1997			308	4.661			1.00	21.47
MOTA	1998	C	THR THR	308	5.242			1.00	24.53
MOTA	1999		PHE	309	4.806			1.00	16.71
MOTA	2000			309	5.628			1.00	12.56
ATOM	2001 2002			309	5.510				13.01
ATOM	2002			309	4.279				2.00
ATOM	2003		1 PHE		3.052			1.00	2.00
ATOM	2004	را		3.55					

# FIG. 1II

MOTA	2005	CD2	PHE	309	4.328	5.363		1.00	3.00 2.72
MOTA	2006	CE1	PHE	309	1.875	4.957		1.00	2.72
MOTA	2007	CE2	PHE	309	3.161	5.391		1.00	2.00
ATOM	2008	CZ	PHE	309	1.925	5.187	1.281		14.67
MOTA	2009	C	PHE	309	7.063	6.949	-1.942		21.23
MOTA	2010	0	PHE	309	7.671	7.453	-1.003 -3.102		16.62
MOTA	2011	N	PRO	310	7.658	6.661	-4.133		15.13
MOTA	2012	CD	PRO	310	7.386	5.631	-3.158		13.22
ATOM	2013	CA	PRO	310	9.053	7.110	-4.256	1.00	12.65
MOTA	2014	CB	PRO	310	9.676	6.241	-5.108	1.00	7.98
MOTA	2015	CG	PRO	310	8.523	5.838 8.630	-3.382	1.00	13.94
MOTA	2016	С	PRO	310	9.143	9.216	-3.302	1.00	16.27
MOTA	2017	0	PRO	310	10.226 7.996	9.257	-3.628	1.00	15.44
MOTA	2018	N	LYS	311		10.708	-3.781	1.00	15.60
MOTA	2019	CA	LYS	311	7.935	11.132	-4.707	1.00	17.57
MOTA	2020	CB	LYS	311	6.795 7.044	10.862	-6.190	1.00	26.47
MOTA	2021	CG	LYS	311	8.243	11.638	-6.731	1.00	31.84
MOTA	2022	CD	LYS	311	8.438	11.399	-8.232	1.00	36.14
MOTA	2023	CE	LYS	311	9.587	12.165	-8.813	1.00	36.37
MOTA	2024	NZ	LYS	311	7.681	11.225	-2.363	1.00	18.67
MOTA	2025	C	LYS	311	8.301	12.192	-1.925	1.00	21.81
MOTA	2026	0	LYS	311 312	6.793	10.534	-1.641	1.00	18.78
MOTA	2027	N	LEU	312	6.451	10.864	-0.254	1.00	13.83
MOTA	2028	CA	LEU	312	5.289	10.003	0.240	1.00	2.00
MOTA	2029	CB	LEU LEU	312	3.891	10.286	-0.301	1.00	2.00
ATOM	2030	CG	LEU	312	2.882	9.395	0.370	1.00	2.00
MOTA	2031	CD1		312	3.540	11.718	-0.037	1.00	3.52
MOTA	2032		LEU	312	7.655	10.637	0.667	1.00	15.47
MOTA	2033	C O	LEU	312	7.805	11.348	1.666	1.00	19.46
MOTA	2034	N	PHE	313	8.491	9.656	0.329	1.00	13.49
MOTA	2035 2036	CA	PHE		9.683	9.326	1.118	1.00	14.43
MOTA	2037	CB	PHE	313	9.434	8.124	2.047	1.00	10.04
MOTA MOTA	2038	CG	PHE	313	8.287	8.327	2.997	1.00	7.55
MOTA	2039		L PHE	313	7.020	7.843	2.679	1.00	4.93
MOTA	2040		PHE	313	8.458	9.044	4.179	1.00	2.84
ATOM	2041		L PHE	313	5.920	8.074	3.505	1.00	2.00
ATOM	2042	CE		313	7.376	9.288	5.021	1.00	2.00
ATOM	2043	CZ	PHE	313	6.094	8.803	4.684	1.00	4.98
ATOM	2044	C	PHE	313	10.896	9.045	0.234	1.00	15.60
MOTA	2045		PHE	313	11.217	7.897	-0.056	1.00	23.18
MOTA	2046		PRO	314	11.573	10.102	-0.217	1.00	14.26
MOTA	2047		PRO	314	11.109	11.483	-0.006	1.00	17.51 17.53
ATOM	2048	CA	PRO	314	12.763	10.085	-1.067	1.00	
ATOM	2049	CB	PRO	314	13.096	11.578		1.00	15.23 13.83
ATOM	2050		PRO	314	11.767	12.228		1.00	19.49
ATOM	2051	. C	PRO	314	13.937	9.357		1.00	20.42
MOTA	2052	0	PRO	314	14.018	9.240			22.24
MOTA	2053	N	ASP	315	14.877	8.924			27.08
MOTA	2054	. CA	ASP	315	16.082	8.238			36.01
MOTA	2055	CB	ASP	315	16.718	7.447			
MOTA	2056			315	16.063	6.099			_
MOTA	2057	7 OD	1 ASP	315	15.166				
MOTA	2058	3 OD	2 ASP	315	16.449				
MOTA	2059		ASP	315	17.099				
MOTA	2060		ASP	315	18.221				
MOTA	2063		SER	316	16.736				
MOTA	2062			316	17.583				
MOTA	2063	3 CE	SER	316	17.239	14.090	, -0.23.		



#### FIG. 1JJ

ATOM	2064	OG	SER	316	15.835	13.079	-0.336		14.43
MOTA	2065	C	SER	316	17.360	11.549	1.866		16.95
ATOM	2066	0	SER	316	18.211	11.999	2.625		19.02 11.69
ATOM	2067	N	LEU	317	16.191	11.062	2.273		10.42
MOTA	2068	CA	LEU	317	15.827	10.956	3.671	1.00	6.04
MOTA	2069	CB	LEU	317	14.329	10.732	3.816	1.00	7.50
ATOM	2070	CG	LEU	317	13.428	11.848	3.325 3.602	1.00	2.00
MOTA	2071		LEU	317	11.977	11.478		1.00	9.21
MOTA	2072		LEU	317	13.826	13.131	4.033 4.306	1.00	14.46
ATOM	2073	C	LEU	317	16.546	9.771 9.876	5.432	1.00	22.75
MOTA	2074	0	LEU	317	17.018	8.643	3.596	1.00	14.45
MOTA	2075	N	PHE	318	16.581 17.224	7.424	4.083	1.00	10.89
MOTA	2076	CA	PHE	318	16.590	6.191	3.452	1.00	6.43
ATOM	2077	CB	PHE	318	15.095	6.168	3.504	1.00	2.63
MOTA	2078	CG	PHE	318	14.351	6.728	2.482	1.00	2.00
MOTA	2079		PHE	318 318	14.431	5.531	4.544	1.00	7.53
MOTA	2080		PHE	318	12.958	6.658	2.479	1.00	2.00
ATOM	2081		PHE PHE	318	13.034	5.450	4.561	1.00	6.05
ATOM	2082		PHE	318	12.294	6.017	3.517	1.00	3.68
MOTA	2083	CZ C	PHE	318	18.689	7.388	3.700	1.00	15.81
MOTA	2084 2085	0	PHE	318	19.110	8.087	2.789	1.00	24.20
MOTA		N	PRO	319	19.505	6.625	4.443	1.00	17.34
MOTA	2086 2087	CD	PRO	319	19.258	6.115	5.805	1.00	13.79
MOTA MOTA	2088	CA	PRO	319	20.931	6.546	4.089	1.00	20.27
ATOM	2089	CB	PRO	319	21.579	6.029	5.378	1.00	19.75
ATOM	2090	CG	PRO	319	20.472	5.258	6.058	1.00	15.80
ATOM	2091	c	PRO	319	21.077	5.556	2.913	1.00	24.31
ATOM	2092	ō	PRO	319	20.155	4.782	2.648	1.00	21.99
ATOM	2093	N	ALA	320	22.196	5.599	2.185	1.00	26.79
ATOM	2094	CA	ALA	320	22.375	4.695	1.045	1.00	27.80
ATOM	2095	CB	ALA	320	21.552	5.183	-0.148	1.00	27.57
MOTA	2096	С	ALA	320	23.818	4.473	0.620	1.00	29.97 25.49
ATOM	2097	0	ALA	320	24.100	4.274	-0.561	1.00	34.44
ATOM	2098	N	ASP	321	24.738	4.488	1.575	1.00 1.00	38.90
ATOM	2099	CA	ASP	321	26.145	4.267	1.246	1.00	42.26
MOTA	2100	CB	ASP	321	27.056	4.965	2.269 3.672	1.00	48.36
MOTA	2101	CG	ASP	321	26.867	4.424	4.293	1.00	50.98
MOTA	2102		1 ASP	321	25.821	4.724	4.144	1.00	52.03
MOTA	2103		2 ASP	321	27.759		1.195	1.00	37.24
MOTA	2104	C	ASP	321	26.445		1.349	1.00	36.84
MOTA	2105		ASP	321	27.601		0.994	1.00	28.45
MOTA	2106		SER	322	25.404		0.924	1.00	25.68
MOTA	2107			322	25.560 25.780		2.322	1.00	27.15
MOTA	2108			322	24.576		3.078		23.17
MOTA	2109			322	24.345				22.83
MOTA	2110		SER	322 322	23.264			1.00	23.80
MOTA	2111		SER	323	24.505			1.00	18.89
MOTA	2112		GLU	323	23.406			1.00	18.36
MOTA	2113			323	23.899			1.00	
MOTA	2114			323	23.139				
MOTA	2115 2116			323	23.509		-3.674		
MOTA			E1 GLU	323	24.719		-3.918	1.00	
MOTA	2117 2118		E2 GLU	323	22.591		-4.332		
MOTA MOTA	2110		GLU GLU	323	22.400	-2.498	0.465		
ATOM	2120		GLU		21.194				
ATOM	212		HIS	324	22.913	3 -2.648			
MOTA	212			324	22.09		2.868	3 1.00	12.46
AIOM	د عـ د. د.	_ ~							



# FIG. 1KK

										10.00
MOTA	2123	CB	HIS	324		22.981	-3.132	4.105 5.366	1.00	18.88 19.65
ATOM	2124		HIS	324		22.200	-3.360	5.845	1.00	15.42
MOTA	2125	CD2		324		21.581	-4.464 -2.347	6.261	1.00	19.17
MOTA	2126	ND1		324		21.924	-2.815	7.230	1.00	20.86
MOTA	2127	CE1		324		21.160 20.937	-4.097	7.003	1.00	17.26
MOTA	2128		HIS	324		20.937	-1.782	3.115	1.00	11.45
ATOM	2129	C	HIS	324		19.954	-1.980	3.338	1.00	12.09
MOTA	2130	0	HIS	324 325		21.689	-0.568	3.065	1.00	12.08
MOTA	2131	N	ASN .	325 325		20.875	0.626	3.278	1.00	15.82
ATOM	2132	CA	asn asn	325		21.758	1.876	3.403	1.00	18.70
MOTA	2133	CB CG	ASN	325		22.479	1.960	4.746	1.00	14.57
ATOM	2134 2135		ASN	325		21.934	1.558	5.777	1.00	20.65
MOTA	2136		ASN	325		23.702	2.489	4.742	1.00	8.45
MOTA	2137	C	ASN	325		19.820	0.802	2.186	1.00	17.97
MOTA MOTA	2138	Ö	ASN	325		18.671	1.166	2.474	1.00	18.10
MOTA	2139	И	LYS	326		20.197	0.498	0.943	1.00	17.49
MOTA	2140	CA	LYS	326		19.279	0.599	-0.189	1.00	13.39
ATOM	2141	CB	LYS	326		20.015	0.328	-1.496	1.00	13.97
ATOM	2142	CG	LYS	326		20.891	1.471	-1.948	1.00	13.26
ATOM	2143	CD	LYS	326		21.753	1.047	-3.118	1.00	16.38
ATOM	2144	CE	LYS	326		22.596	2.202	-3.628	1.00	18.48
ATOM	2145	NZ	LYS	326		23.721	1.752	-4.511	1.00	20.03
ATOM	2146	C	LYS	326		18.111	-0.367	-0.043	1.00	12.95
ATOM	2147	0	LYS	326		16.955	0.008	-0.263	1.00	17.37
ATOM	2148	N	LEU	327		18.402	-1.599	0.365	1.00	8.13
MOTA	2149	CA	LEU	327		17.362	-2.605	0.549	1.00	6.10 10.78
MOTA	2150	CB	LEU	327		17.992	-3.973	0.798	1.00 1.00	5.81
ATOM	2151	CG	LEU	327		17.045	-5.113	1.171	1.00	8.81
MOTA	2152		LEU	327		16.166	-5.466	-0.012 1.610	1.00	2.24
MOTA	2153	CD2		327		17.852	-6.305 -2.251	1.708	1.00	7.31
MOTA	2154	C	LEU	327		16.438	-2.409	1.609	1.00	9.49
MOTA	2155	0	LEU	327		15.217	-1.785	2.809	1.00	5.63
MOTA	2156	N	LYS	328		17.026 16.252	-1.402	3.985	1.00	5.88
MOTA	2157	CA	LYS	328 328		17.166	-1.179	5.191	1.00	10.06
MOTA	2158	CB	LYS	328		17.780	-2.465	5.720	1.00	11.60
ATOM	2159	CG	LYS LYS	328		16.679	-3.468	6.024	1.00	8.26
ATOM	2160	CD	LYS	328		17.231	-4.789	6.516	1.00	7.01
MOTA	2161 2162	NZ	LYS	328		16.118	-5.682	6.946	1.00	9.67
MOTA MOTA	2163	C	LYS	328		15.422	-0.165	3.725	1.00	5.26
ATOM	2164	o	LYS	328		14.284	-0.064	4.193	1.00	5.47
ATOM	2165	N	ALA	329		15.981	0.763	2.954	1.00	4.26
ATOM	2166		ALA	329		15.291	1.997	2.624	1.00	5.46
ATOM	2167	CB	ALA	329		16.196	2.911	1.825	1.00	8.76
ATOM	2168	C	ALA	329		14.024	1.676	1.845	1.00	8.00
ATOM	2169	ō	ALA	329		12.987	2.308	2.054	1.00	12.88
ATOM	2170	N	SER	330		14.095	0.665	0.975	1.00	12.20
ATOM	2171	CA		330		12.933	0.244	0.184	1.00	12.36
MOTA	2172	CB	SER	330		13.363	-0.524	-1.070	1.00	14.81
ATOM	2173	OG	SER	330		14.281		-0.770	1.00	19.19
ATOM	2174	С	SER	330		11.929		1.019	1.00	9.23 9.24
MOTA	2175	0	SER	330		10.715		0.841		14.64
MOTA	2176	N	GLN	331		12.439		1.966		
MOTA	2177			331		11.580		2.861		
MOTA	2178			331		12.409		3.608		_
MOTA	2179			331		12.776		2.764 3.417		
MOTA	2180					13.811		4.232		
MOTA	2181	. OE	1 GLN	331	,	14.614	-4.008	T.434	1.00	_,



## FIG. 1LL

								1 00	24.53
MOTA	2182	NE2	GLN	331	13.811	-6.577	3.037		10.18
MOTA	2183	_	GLN	331	10.835	-1.211	3.851		11.53
MOTA	2184	0 .	GLN	331	9.673	-1.460	4.199 4.275	1.00	6.48
MOTA	2185	N	ALA	332	11.490	-0.135	5.194	1.00	4.04
MOTA	2186	CA	ALA	332	10.876	0.809	5.605	1.00	2.00
MOTA	2187	CB	ALA	332	11.871	1.849	4.451	1.00	10.26
MOTA	2188	C	ALA	332	9.734	1.456	4.900	1.00	10.60
MOTA	2189	0	ALA	332	8.584	1.433	3.246	1.00	15.77
MOTA	2190	N	ARG	333	10.055	1.927	2.351	1.00	13.48
MOTA	2191	CA	ARG	333	9.110	2.584	1.104	1.00	14.31
MOTA	2192	CB	ARG	333	9.848	3.065 3.999	0.204	1.00	12.38
MOTA	2193	CG	ARG	333	9.063	4.319	-1.017	1.00	11.06
MOTA	2194	CD	ARG	333	9.895	5.055	-0.679	1.00	10.28
MOTA	2195	NE	ARG	333	11.106		-1.194	1.00	17.30
MOTA	2196	$\mathbf{cz}$	ARG	333	12.307	4.814	-2.082	1.00	23.65
MOTA	2197	NH1	ARG	333	12.477	3.847	-0.809	1.00	18.12
MOTA	2198	NH2	ARG	333	13.350	5.539	1.984	1.00	13.96
MOTA	2199	C	ARG	333	7.979	1.620	1.867	1.00	15.40
MOTA	2200	0	ARG	333	6.823	2.038	1.854	1.00	10.58
MOTA	2201	N	ASP	334	8.300	0.328 -0.696	1.538	1.00	11.35
MOTA	2202	CA	ASP	334	7.302		1.211	1.00	20.54
MOTA	2203	CB	ASP	334	7.970	-2.037	0.915	1.00	24.07
MOTA	2204	CG	ASP	334	6.956	-3.141	0.046	1.00	30.63
ATOM	2205		ASP	334	6.077	-2.941	1.553	1.00	26.21
MOTA	2206		ASP	334	7.037	-4.213	2.722	1.00	9.90
MOTA	2207	C	ASP	334	6.358	-0.877	2.722	1.00	10.84
MOTA	2208	0	ASP	334	5.140	-0.961	3.920	1.00	9.79
MOTA	2209	N	LEU	335	6.922	-0.950	5.116	1.00	8.58
MOTA	2210	CA	PEA	335	6.111	-1.095 -1.148	6.335	1.00	11.28
ATOM	2211	CB	LEU	335	7.019	-1.148	7.728	1.00	7.73
MOTA	2212	CG	LEU	335	6.454 5.444	-2.553	7.731	1.00	4.16
MOTA	2213		LEU	335	7.624	-1.740	8.626	1.00	6.63
MOTA	2214	CD2		335	5.173	0.099	5.197	1.00	6.79
MOTA	2215	C	LEU	335	3.965	-0.062	5.362	1.00	8.39
MOTA	2216	0	LEU	335	5.738	1.287	4.993	1.00	4.95
MOTA	2217	N	LEU	336	4.996	2.548	5.016	1.00	5.17
ATOM	2218	CA	LEU	336	5.933	3.713	4.691	1.00	2.00
MOTA	2219	CB	LEU	336	6.763	4.238	5.867	1.00	3.17
MOTA	2220	CG	LEU	336	8.067		5.418	1.00	2.00
MOTA	2221	CDI		336	5.907		6.658	1.00	2.00
MOTA	2222	CD2		336 336	3.829		4.044	1.00	7.82
MOTA	2223	C	LEU	336	2.728		4.380	1.00	7.70
ATOM	2224	0	LEU	337	4.061		2.861	1.00	12.67
MOTA	2225		SER		3.035		1.831	1.00	16.08
MOTA	2226		SER	337	3.653		0.524	1.00	17.25
MOTA	2227		SER	337	3.994		0.602	1.00	16.83
MOTA	2228		SER	337	1.909		2.245	1.00	17.26
MOTA	2229		SER	337	0.786		1.743	1.00	19.04
MOTA	2230		SER	337	2.227		3.128	1.00	17.99
MOTA	2231		LYS	338	1.256		3.617		10.96
MOTA	2232			338	1.965		4.091		12.91
MOTA	2233			338	2.830		3.070	_	11.53
MOTA	2234			338	2.082		2.357		11.57
MOTA	2235				3.033		2.000		17.59
MOTA	2236				4.347		1.464		5.95
ATOM	2237								6.87
MOTA	2238		LYS		0.460				
MOTA	2239		LYS		-0.737	·			
MOTA	2240	) N	MET	339	1.128	, 0.202			

## FIG. 1MM

						0.040	6.833	1.00	12.64
MOTA	2241	CA	MET	339	0.476	0.842 1.161	7.921		13.33
ATOM	2242	CB	MET	339	1.505		8.514	1.00	13.21
MOTA	2243	CG	MET	339	2.181	-0.061 0.357	9.675	1.00	17.84
MOTA	2244	SD	MET	339	3.475		10.884	1.00	20.59
MOTA	2245	CE	MET	339	3.218		6.530	1.00	10.81
MOTA	2246	C	MET	339	-0.347	2.082 2.168	6.930	1.00	11.79
MOTA	2247	0	MET	339	-1.512		5.813	1.00	10.89
ATOM	2248	N	LEU	340	0.257	3.029	5.454	1.00	9.27
MOTA	2249	CA	LEU	340	-0.415	4.271 5.366	5.118	1.00	7.51
MOTA	2250	CB	LEU	340	0.598	5.939	6.344	1.00	7.71
MOTA	2251	CG	LEU	340	1.311	6.771	5.938	1.00	7.14
MOTA	2252		LEU	340	2.511	6.747	7.179	1.00	6.71
MOTA	2253		<b>LEU</b>	340	0.336	4.082	4.310	1.00	10.12
MOTA	2254	С	LEU	340	-1.390 -1.132	4.510	3.187	1.00	13.32
MOTA	2255	0	LEU	340	-2.528	3.465	4.624	1.00	5.63
MOTA	2256	N	VAL	341	-2.526	3.205	3.656	1.00	4.39
MOTA	2257	CA	VAL	341	-3.561	1.693	3.360		7.19
MOTA	2258	CB	VAL	341	-3.669 -4.868	1.408	2.461	1.00	8.69
MOTA	2259		VAL	341	-4.868	1.195	2.714	1.00	8.14
MOTA	2260		VAL	341	-4.891	3.718	4.227	1.00	5.17
ATOM	2261	C	VAL	341	-5.314	3.728	5.290	1.00	15.43
MOTA	2262	0	VAL	341	-5.557	4.599	3.491	1.00	6.54
MOTA	2263	N	ILE	342	-6.812	5.218	3.922	1.00	8.56
MOTA	2264	CA	ILE	342	-7.260	6.324	2.923	1.00	7.43
MOTA	2265	CB	ILE	342	-8.616	6.906	3.297	1.00	2.37
MOTA	2266		ILE	342	-6.209	7.432	2.881	1.00	10.85
MOTA	2267		ILE	342	-6.577	8.551	1.933	1.00	13.32
MOTA	2268		ILE	342	-7.947	4.244	4.159	1.00	12.09
MOTA	2269	C	ILE	342	-8.858	4.534	4.930	1.00	18.08
MOTA	2270	0	ILE	342 343	-7.910	3.097	3.500	1.00	19.41
MOTA	2271	N	ASP	343	-8.972	2.117	3.688	1.00	20.62
MOTA	2272	CA	ASP	343	-9.398	1.538	2.336	1.00	23.24
MOTA	2273	CB	ASP ASP	343	-10.671	0.714	2.422	1.00	24.40
MOTA	2274	CG	ASP 1 ASP	343	-11.556	1.024	3.248	1.00	28.91
MOTA	2275		2 ASP	343	-10.805	-0.243	1.638	1.00	33.68
ATOM	2276		Z ASP ASP	343	-8.516	1.006	4.630	1.00	20.89
ATOM	2277	C	ASP	343	-7.448	0.417	4.446	1.00	24.41
ATOM	2278	0	PRO	344	-9.295	0.747	5.686	1.00	18.88
MOTA	2279	И		344	-10.522	1.442	6.107	1.00	18.84
MOTA	2280	CD		344	-8.952	-0.306	6.641	1.00	17.35
MOTA	2281	CA CB		344	-10.148	-0.290	7.595	1.00	16.82
ATOM	2282			344	-10.594	1.118	7.571	1.00	9.78
ATOM	2283		PRO	344	-8.865	-1.640	5.917	1.00	19.67
MOTA	2284 2285		PRO	344	-7.942	-2.422	6.152	1.00	20.89
MOTA			ALA	345	-9.811		4.992	1.00	
MOTA	2286			345	-9.916		4.192	1.00	
MOTA	2287 2288			345	-11.200		3.363	1.00	9.24
MOTA			ALA		-8.726		3.301	1.00	
MOTA	2289		ALA		-8.619		2.781	1.00	
MOTA	2290		LYS	346	-7.853		3.098	1.00	
MOTA	2291 2292				-6.661		2.288		
MOTA	2293				-6.628		1.122		
MOTA					-7.759				
MOTA MOTA	2294 2295				-7.699				
MOTA	2296				-8.808				
ATOM	2297				-8.612		-2.792		
ATOM	2298		LYS		-5.428				
MOTA			LYS		-4.313		2.722	2 1.00	14.60
ALOM	4433	, ,		240					

## FIG. 1NN

ATOM	2300	N	ARG	347	-	5.637	-2.018	4.403	1.00	18.46
ATOM	2301	CA	ARG	347	-	4.544	-1.820	5.352	1.00	15.01
MOTA	2302	CB	ARG	347	-	4.935	-0.811	6.433	1.00	13.75
MOTA	2303	CG	ARG	347	•	-3.733	-0.158	7.128	1.00	9.99
MOTA	2304	CD	ARG	347	•	-4.175	0.743	8.272	1.00	8.39
MOTA	2305	NE	ARG	347		-5.122	1.755	7.812	1.00	11.90
ATOM	2306	$\mathbf{C}\mathbf{Z}$	ARG	347		-6.130	2.242	8.529	1.00	14.87
ATOM	2307	NH1	ARG	347		-6.350	1.821	9.765	1.00	20.10
ATOM	2308	NH2	ARG	347		-6.945	3.137	7.995	1.00	13.60
ATOM	2309	С	ARG	347		-4.074	-3.133	6.003	1.00	15.98
MOTA	2310	0	ARG	347		-4.868	-4.024	6.321	1.00	18.25
MOTA	2311	N	ILE	348		-2.764	-3.221	6.204	1.00	12.17
MOTA	2312	CA	ILE	348		-2.088	-4.367	6.802	1.00	10.44
MOTA	2313	CB	ILE	348		-0.556	-4.152	6.681	1.00	2:00
ATOM	2314	CG2	ILE	348		-0.095	-3.082	7.655	1.00	4.05
ATOM	2315	CG1	ILE	348		0.198	-5.444	6.951	1.00	2.00
ATOM	2316	CD1	ILE	348		1.708	-5.293	6.822	1.00	3.75
MOTA	2317	С	ILE	348		-2.444	-4.519	8.286	1.00	15.07
ATOM	2318	0	ILE	348		-2.906	-3.565	8.912	1.00	24.64
MOTA	2319	N	SER	349		-2.222	-5.708	8.848	1.00	17.85
ATOM	2320	CA	SER	349		-2.500	-5.961	10.265	1.00	12.24
ATOM	2321	CB	SER	349		-3.243	-7.288	10.435	1.00	18.76
ATOM	2322	OG	SER	349		-2.400	-8.380	10.114	1.00	24.15
ATOM	2323	С	SER	349		-1.202	-5.990	11.093	1.00	13.20
MOTA	2324	0	SER	349		-0.089	-5.901	10.548	1.00	8.49
MOTA	2325	N	VAL	350		-1.353	-6.169	12.407	1.00	11.30
ATOM	2326	CA	VAL	350		-0.226	-6.196	13.338	1.00	4.95
ATOM	2327	CB	VAL	350		-0.711	-6.298	14.829	1.00	11.43
ATOM	2328	CG1	VAL	350		0.454	-6.071	15.780	1.00	8.45
ATOM	2329	CG2	VAL	350		-1.822	-5.269	15.122	1.00	7.42
MOTA	2330	C	VAL	350		0.732	-7.336	13.037	1.00	2.00
MOTA	2331	0	VAL	350		1.951	-7.153	12.998	1.00	2.70
ATOM	2332	N	ASP	351		0.192	-8.513	12.763	1.00	8.23
ATOM	2333	CA	ASP	351		1.059	-9.648	12.484	1.00	10.61
MOTA	2334	CB	ASP	351		0.284	-10.952	12.555	1.00	18.49
MOTA	2335	CG	ASP	351		0.210	-11.491	13.964	1.00	18.11
ATOM	2336	OD1	ASP	351			-11.903	14.470	1.00	22.45
ATOM	2337		ASP	351		-0.899	-11.495	14.546	1.00	14.05
ATOM	2338	С	ASP	351		1.863	-9.567	11.212	1.00	9.41
ATOM	2339	0	ASP	351		3.064	-9.841	11.221	1.00	11.00
MOTA	2340	N	ASP	352		1.222	-9.189	10.114	1.00	10.25
ATOM	2341	CA	ASP	352		1.950	-9.069	8.857	1.00	12.98
ATOM	2342	CB	ASP	352		1.010	-8.664	7.725	1.00	10.96
ATOM	2343	CG	ASP	352		-0.227	-9.525	7.649	1.00	12.21
MOTA	2344	OD:	1 ASP	352		-0.131	-10.756	7.855	1.00	12.96
ATOM	2345		2 ASP	352		-1.303	-8.959	7.374	1.00	15.38
ATOM	2346		ASP	352		3.018	-7.994	9.045	1.00	15.26
ATOM	2347		ASP	352		4.150	-8.133	8.569	1.00	18.07
ATOM	2348		ALA	353		2.660	-6.958	9.805	1.00	14.96
ATOM	2349			353		3.552	-5.846	10.092	1.00	10.83
ATOM	2350			353		2.796	-4.737	10.805		14.35
MOTA	2351		ALA	353		4.734	-6.332	10.927		10.55
MOTA	2352		ALA	353		5.864	-5.892	10.716		10.08
ATOM	2353		LEU	354		4.481	-7.282	11.831		10.79
ATOM	2354			354		5.529		12.683		7.58
ATOM	2355			354		4.917	-8.549	13.900		8.36
MOTA	2356			354		4.569	-7.702	15.136		
MOTA	2357		1 LEU	354		3.437		15.905		
MOTA	2358		2 LEU	354		5.789	-7.506	16.029	1.00	2.00



# FIG. 100

					<i>-</i> 1	00	-8.824	11.906	1.00	7.39
MOTA			LEU	354	6.4		-8.906	12.116	1.00	2.00
MOTA	2360		LEU	354	7.6		-9.534	10.979	1.00	9.55
MOTA			GLN	355	5.7		-10.522	10.144		L3.96
MOTA	2362	CA	GLN	355	6.4			9.672		L3.47
ATOM	2363	CB	GLN	355	5.4		-11.586	10.767		12.65
MOTA	2364	CG	GLN	355	4.8	48	-12.460	11.003		19.49
ATOM	2365	CD	GLN	355			-13.716		-	21.81
ATOM	2366	OE1	GLN	355	6.8	37	-13.668	11.318	1.00	21.15
MOTA	2367	NE2	GLN	355			-14.859	10.842		15.16
MOTA	2368	C .	GLN	355	7.1		-9.893	8.925	_	16.20
ATOM	2369	0	GLN	355			-10.561	8.228	_	15.76
ATOM	2370	N	HIS	356	6.8		-8.614	8.675	1.00	9.95
ATOM	2371	CA	HIS	356	7.3		-7.889	7.530		7.19
ATOM	2372	CB	HIS	356	-	317	-6.469	7.534	1.00	5.18
ATOM	2373	CG	HIS	356	7.3	L75	-5.666	6.320	1.00	2.47
MOTA	2374		HIS	356	6.4	126	-5.261	5.277	1.00	
ATOM	2375		HIS	356	8.4	457	-5.216	6.076	1.00	3.37
MOTA	2376		HIS	356	8.4	481	-4.577	4.923	1.00	8.01
ATOM	2377		HIS	356	7.3	261	-4.587	4.416	1.00	9.88
ATOM	2378	C	HIS	356	8.	922	-7.838	7.558	1.00	11.50
	2379	ō	HIS	356	9.	501	-7.569	8.597	1.00	15.45
MOTA	2380	N	PRO	357	9.	593	-8.064	6.409	1.00	14.61
MOTA	2381	CD	PRO	357	8.	977	-8.395	5.114	1.00	16.32
MOTA	2381	CA	PRO	357	11.	065	-8.045	6.276	1.00	12.00
MOTA	2382	CB	PRO	357	11.	287	-8.137	4.756	1.00	14.38
MOTA		CG	PRO	357	9.	955	-7.764	4.152	1.00	16.33
MOTA	2384	C	PRO	357		821	-6.863	6.889	1.00	13.41
MOTA	2385		PRO	357		036		7.112	1.00	16.91
MOTA	2386	О И	TYR	358		140		7.113	1.00	15.19
MOTA	2387		TYR	358		778		7.737	1.00	16.88
MOTA	2388	CA CB	TYR	358		053		7.379	1.00	11.17
ATOM	2389		TYR	358		801		7.881	1.00	7.46
ATOM	2390	CG	LTYR	358		148		7.585	1.00	5.18
MOTA	2391	CE1		358		870		8.112	1.00	8.86
MOTA	2392			358		193		8.718	1.00	9.39
MOTA	2393	CD2		358		918		9.252	1.00	2.00
MOTA	2394	CE	TYR	358		. 255	_	8.944	1.00	4.61
ATOM	2395	CZ		358		.007			1.00	4.98
MOTA	2396	OH	TYR	358		.781	_		1.00	17.22
MOTA	2397	C.	TYR	358		. 697	_		1.00	16.24
MOTA	2398	0	TYR	359		.772	_		1.00	16.60
MOTA	2399		· ILE	359		.589			1.00	14.11
MOTA	2400			359		. 093			1.00	16.20
MOTA	2401			359		.878			1.00	19.56
MOTA	2402					.56			1.00	5.87
MOTA	2403		1 ILE	359		.25				13.16
MOTA	2404	-	1 ILE	359		.02	_			15.39
MOTA	2405		ILE	359		.67	-			16.24
MOTA	2406		ILE	359		.68				14.64
MOTA	2407		ASN	360						9.97
MOTA	2408			360	10	.98	4 -10.49	_		7.20
MOTA	2409			360	10	1.44	3 -10.50			3.95
MOTA	2410			360	11	. IJ	9 -10.38	_		2.00
MOTA	2411		1 ASN	360	12	. 35	9 -10.38			2.26
MOTA	2412	S NE	2 ASN							13.06
MOTA	2413	3 C	ASN			.40				
MOTA	2414	1 0	ASN				0 -10.96			
MOTA	241	5 N	VAL			3.38				
MOTA	2416	S CI				1.74				
MOTA		7 CI	3 VAL	361	15	5.81	.2 -8.27			



## FIG. 1PP

ATOM	2418	CG1	VAL	361	15	.998	-8.423	10.277		23.78
ATOM	2419	CG2	VAL	361		.412	-6.860	12.104		11.95
MOTA	2420	C.	VAL	361		.829	-9.400	13.803		24.53 28.66
MOTA	2421	0	VAL	361			-10.048	14.341	1.00	23.87
MOTA	2422	N	TRP	362		3.886	-8.758	14.496 15.960	1.00	18.58
MOTA	2423	CA	TRP	362		3.835	-8.778 -7.392	16.521	1.00	12.66
MOTA	2424	CB	TRP	362		3.483 1.272	-6.282	15.991	1.00	4.45
MOTA	2425	CG	TRP	362		5.653	-6.011	16.254	1.00	4.23
MOTA	2426		TRP TRP	362 362		5.987	-4.843	15.536	1.00	2.00
ATOM	2427		TRP	362		5.631	-6.646	17.017	1.00	2.00
ATOM ATOM	2428 2429	CD1		362		3.836	-5.301	15.162	1.00	2.00
MOTA	2430		TRP	362		4.860	-4.431	14.881	1.00	2.00
MOTA	2431	CZ2		362	1	7.270	-4.289	15.568	1.00	2.00
ATOM	2432	CZ3	TRP	362	1	7.901	-6.100	17.051	1.00	7.07
ATOM	2433	CH2	TRP	362	1	8.212	-4.930	16.324	1.00	8.63
MOTA	2434	C	TRP	362		2.742	-9.730	16.425	1.00	20.11
MOTA	2435	0	TRP	362		2.514	-9.871	17.626	1.00	19.34 15.68
ATOM	2436	N	TYR	363			-10.363	15.488	1.00 1.00	12.75
MOTA	2437	CA	TYR	363			-11.246	15.851 14.611	1.00	4.47
MOTA	2438	CB	TYR	363			-11.853 -12.294	14.820	1.00	7.70
MOTA	2439	CG	TYR	363			-13.571	15.297	1.00	6.58
MOTA	2440	CD1		363			-13.975	15.468	1.00	2.00
MOTA	2441	CE1		363 363			-11.441	14.523	1.00	2.00
MOTA	2442	CD2		363			-11.836	14.688	1.00	5.09
MOTA	2443 2444	CEZ	TYR	363			-13.100	15.158	1.00	4.18
ATOM	2444	OH	TYR	363		4.898	-13.484	15.291	1.00	15.76
MOTA MOTA	2446	C	TYR	363	ב		-12.336	16.812	1.00	16.54
MOTA	2447	ō	TYR	363			-13.057	16.556	1.00	20.38
ATOM	2448	N	ASP	364			-12.380	17.962	1.00	15.31
ATOM	2449	CA	ASP	364			3 -13.366	18.999	1.00	10.29
MOTA	2450	CB	ASP	364			3 -12.765	20.134	1.00	12.82 13.30
MOTA	2451	CG	ASP	364	=	L2.149	-13.764	21.222	1.00 1.00	11.59
MOTA	2452		L ASP	364			5 -14.281	21.823 21.472	1.00	14.16
MOTA	2453		2 ASP	364	-		7 -14.040 3 -13.658	19.458	1.00	9.97
MOTA	2454	С	ASP	364			9 -12.772	19.943	1.00	14.45
MOTA	2455	0	ASP	364			B -14.907		1.00	9.41
MOTA	2456	И	PRO	365		9.88			1.00	3.16
MOTA	2457	CD	PRO	365 365		7.80			1.00	5.93
MOTA	2458	CA CB	PRO PRO	365			6 -16.668		1.00	2.73
MOTA MOTA	2459 2460			365			1 -17.222		1.00	2.00
ATOM	2461		PRO	365			2 -15.053	21.217	1.00	5.07
ATOM	2462		PRO	365			9 ~15.029		1.00	3.26
ATOM	2463		ALA	366			9 -14.888		1.00	5.56
ATOM	2464		ALA	366			2 -14.690		1.00	13.27
ATOM	2465		ALA	366			9 -14.902			16.70 14.41
MOTA	2466	C	ALA	366			8 -13.284			19.61
MOTA	2467	0	ALA	366	-		2 -13.107			15.02
ATOM	2468		GLU	367			5 -12.302			5.43
MOTA	2469			367		9.12	9 -10.883 3 -9.999			2.00
MOTA	2470			367			6 -10.213			
MOTA	2471			367 367		11.56				
MOTA	2472			367 367		12.72				
ATOM	2473		:1 GLU :2 GLU	367 367		11.28		_		
MOTA MOTA	2474 2475		GLU GLU	367			2 -10.59			
ATOM	2476		GLU	367		5.87			1.00	2.04
WIOM	24/6	, 0	اللك	507						

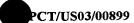


# FIG. 1QQ

								01 015	1 00	7 07
MOTA	2477	N	VAL	368			-11.197 -10.995		1.00 1.00	7.87 7.65
MOTA	2478	CA	VAL	368			-10.995 -11.535			12.19
MOTA	2479	CB	VAL	368			-11.533		1.00	9.04
MOTA	2480		VAL	368			-10.684	18.169	1.00	2.75
ATOM	2481	CG2	VAL	368			-11.656	20.998	1.00	7.96
MOTA	2482	C	VAL	368 368			-11.042	21.109	1.00	15.88
MOTA	2483	0	VAL ALA	369			-12.901	21.428	1.00	17.86
MOTA	2484	N CA	ALA	369			-13.640	22.039	1.00	25.19
MOTA	2485 2486	CB	ALA	369			-15.013	21.382	1.00	23.81.
MOTA	2487	C	ALA	369			-13.774	23.572	1.00	30.10
MOTA MOTA	2488	0	ALA	369			-14.814	24.096	1.00	36.36
ATOM	2489	N	ALA	370			-12.706	24.275	1.00	27.76
MOTA	2490	CA	ALA	370			-12.678	25.731	1.00	23.19
ATOM	2491	CB	ALA	370		3.916	-11.564	26.236	1.00	19.06
ATOM	2492	C	ALA	370			-12.411	26.105	1.00	25.30
MOTA	2493	ō	ALA	370			-11.327	25.856	1.00	28.84
ATOM	2494	N	PRO	371			-13.398	26.695	1.00	30.05
ATOM	2495	CD	. PRO	371			-14.670	27.208	1.00	30.56
MOTA	2496	CA	PRO	371			-13.238	27.085	1.00	30.50
MOTA	2497	CB	PRO	371			-14.618	27.647	1.00	29.26 31.17
MOTA	2498	CG	PRO	371			-15.060	28.275	1.00	29.61
MOTA	2499	C	PRO	371		-0.740	-12.117	28.109	1.00 1.00	28.65
MOTA	2500	0	PRO	371			-11.801	28.895	1.00	29.10
MOTA	2501	N	PRO	372			-11.473	28.065 27.024	1.00	31.05
MOTA	2502	CD	PRO	372			-11.710	28.954	1.00	32.89
MOTA	2503	CA	PRO	372			-10.381	28.208	1.00	26.47
MOTA	2504	CB	PRO	372		-3.551	-11.002	27.577	1.00	27.14
MOTA	2505	CG	PRO	372		-2.733		30.363	1.00	37.35
MOTA	2506	C	PRO	372 372			-11.974	30.476	1.00	41.20
MOTA	2507	0	PRO ALA	382		-17.334		28.970	1.00	45.07
MOTA	2508	CB C	ALA	382		-19.469		30.278	1.00	43.41
MOTA	2509 2510	0	ALA	382		-20.418		29.516	1.00	43.69
MOTA MOTA	2511	N	ALA	382		-18.413	1.010	29.750	1.00	45.59
ATOM	2512	CA	ALA	382		-18.152	2.445	30.082	1.00	44.95
ATOM	2513	N	ALA	383		-19.519	4.055	31.291	1.00	40.49
MOTA	2514	CA		383		-20.721	4.832	31.581	1.00	37.23
ATOM	2515	CB		383		-21.499		32.734	1.00	35.88
ATOM	2516	С	ALA	383		-20.408		31.888	1.00	35.44
MOTA	2517	0	ALA	383		-19.252		32.105	1.00	33.54 33.22
ATOM	2518	N	GLU	384		-21.450		31.885	1.00 1.00	35.14
ATOM	2519	CA	GLU	384		-21.306		32.161	1.00	39.93
ATOM	2520	CB		384		-22.190		31.209 29.712	1.00	44.06
MOTA	2521			384		-21.976			1.00	47.10
MOTA	2522			384		-20.563			1.00	47.81
ATOM	2523		1 GLU	384		-19.986	-		1.00	50.85
ATOM	2524		2 GLU	384		-20.029			1.00	34.52
MOTA	2525		GLU	384		-21.689 -22.774			1.00	33.70
MOTA	2526		GLU	384		-20.783	·			31.42
ATOM	2527		HIS	385		-21.029			_	
MOTA	2528			385 385		-20.07				
ATOM	2529			385		-20.09				_
MOTA	2530 2531		2 HIS	385		-19.11				
MOTA	2531		O1 HIS	385		-21.26			1.00	
ATOM ATOM	2533		E1 HIS	385		-20.98	4 5.492	36.292		
MOTA	2534		E2 HIS	385		-19.69	1 5.380			
ATOM	2535		HÌS	385		-20.86		36.009	1.00	29.29
AION	200	_		3.55	•					

# FIG. 1RR

MOTA	2536	0	HIS	385	-20.400	11.993	35.143	1.00	31.45
ATOM	2537	N	THR	386	-21.234	11.673	37.211	1.00	24.31
ATOM	2538	CA	THR	386	-21.111	13.067	37.594	1.00	17.05
ATOM	2539	CB	THR	386	-22.149	13.439	38.661	1.00	18.48
MOTA	2540	OG1	THR	386	-21.927	12.653	39.835	1.00	26.84
MOTA	2541	CG2	THR	386	-23.557	13.185	38.152	1.00	14.58
MOTA	2542	С	THR	386	-19.713	13.286	38.147	1.00	18.26
MOTA	2543	0	THR	386	-18.908	12.358	38.198	1.00	16.54
MOTA	2544	N	ILE	387	-19.425	14.514	38.560	1.00	22.20
MOTA	2545	CA	ILE	387	-18.127	14.854	39.120	1.00	24.81
MOTA	2546	CB	ILE	387	-18.003	16.371	39.363	1.00	26.15
MOTA	2547	CG2	ILE	387	-16.738	16.690	40.164	1.00	20.29
MOTA	2548		ILE	387	-18.015	17.107	38.023	1.00	26.13
MOTA	2549	CD1	ILE	387	-18.028	18.611	38.164	1.00	30.51
ATOM	2550	С	ILE	387	-17.978	14.144	40.446	1.00	29.13
MOTA	2551	0	ILE	387	-16.919	13.591	40.744	1.00	36.90
ATOM	2552	N	ALA	388	-19.049	14.151	41.235	1.00	28.74
ATOM	2553	CA	ALA	388	-19.028	13.504	42.539	1.00	27.98
MOTA	2554	CB	ALA	388	-20.269	13.869	43.331	1.00	24.16
MOTA	2555	С	ALA	388	-18.913	12.000	42.356	1.00	27.08
MOTA	2556	0	ALA	388	-18.120	11.351	43.035	1.00	28.54
MOTA	2557	N	GLU	389	-19.647	11.461	41.385	1.00	27.57
MOTA	2558	CA	GLU	389	-19.611	10.025	41.102	1.00	25.55
MOTA	2559	CB	GLU	389	-20.753	9.637	40.169	1.00	20.07
MOTA	2560	CG	GLU	389	-22.115	9.902	40.776	1.00	17.01
MOTA	2561	CD	GLU	389	-23.257	9.727	39.794	1.00	22.78
MOTA	2562		GLU	389	-23.013	9.643	38.572	1.00	24.62
MOTA	2563		GLU	389	-24.417	9.690	40.245	1.00	26.31
ATOM	2564	С	GLU	389	-18.265	9.572	40.530	1.00	27.33
MOTA	2565	0	GLU	389	-17.818	8.461	40.819	1.00	35.55
MOTA	2566	N	TRP	390	-17.611	10.438	39.756	1.00	24.95
MOTA	2567	CA	TRP	390	-16.309	10.124	39.179	1.00	22.08
ATOM	2568	CB	TRP	390	-15.975	11.055	37.995	1.00	26.49
MOTA	2569	CG	TRP	390	-16.480	10.612	36.619	1.00	31.67
MOTA	2570	CD2		390	-16.260	9.335	35.968	1.00	29.90
MOTA	2571	CE2		390	-16.914	9.391	34.714	1.00	28.93
MOTA	2572	CE3		390	-15.580	8.164	36.323	1.00	27.49
MOTA	2573	CD1		390	-17.229	11.356	35.747	1.00	31.50
MOTA	2574	NE1		390	-17.493	10.630	34.606	1.00	32.29
MOTA	2575	CZ2		390	-16.903	8.316	33.819	1.00	29.75
MOTA	2576	CZ3		390	-15.569	7.102	35.437	1.00	29.76 31.94
MOTA	2577	CH2		390	-16.229	7.183	34.198	1.00	
MOTA	2578	C	TRP	390	-15.207	10.266	40.227	1.00	21.39
ATOM	2579	0	TRP	390	-14.144	9.661	40.100	1.00	26.37
ATOM	2580	N	LYS	391	-15.453	11.085	41.245	1.00	19.83
MOTA	2581	CA	LYS	391	-14.484	11.323	42.314	1.00	16.84
MOTA	2582	CB	LYS	391	-14.925	12.544	43.132	1.00	14.49
MOTA	2583	CG	LYS	391	-13.951	13.006	44.213	1.00	10.70
MOTA	2584	CD	LYS	391	-14.510	14.218	44.963	1.00	13.44
MOTA	2585	CE	LYS	391	-13.478		45.906	1.00	8.99
MOTA	2586	NZ	LYS	391	-14.038	16.018	46.657	1.00	9.86
MOTA	2587	C	LYS	391	-14.328	10.102	43.231	1.00	18.26
MOTA	2588	0	LYS	391	-13.214	9.769	43.654	1.00	15.87
MOTA	2589	N	GLU	392	-15.451	9.443		. 1.00	20.49
MOTA	2590	CA	GLU	392	-15.483	8.267	44.386	1.00	23.22
MOTA	2591	CB	GLU	392	-16.924	7.953	44.777	1.00	26.59
MOTA	2592	CG	GLU	392	-17.050	6.956	45.911	1.00	36.07
MOTA	2593	CD	GLU		-18.359	7.099	46.663	1.00	41.89
MOTA	2594	OE:	L GLU	392	-18.310	7.239	47.902	1.00	41.27



## FIG. 1SS

		070	CT II	202	-19.432	7.071	46.018	1.00	50.99
MOTA		OE2	GLU	392 392	-14.840	7.052	43.737	1.00	22.68
ATOM		C	GLU	392	-14.103	6.304	44.389		23.88
MOTA	2597	0	LEU	393	-15.137	6.853	42.455	1.00	20.40
ATOM	2598	N CA	LEU	393	-14.583	5.746	41.693	1.00	14.24
MOTA	2599	CB	LEU	393	-15.141	5.763	40.280	1.00	9.57
ATOM	2600 2601	CG	LEU	393	-16.578	5.266	40.243	1.00	13.19
MOTA	2602		LEU	393	-17.203	5.553	38.884	1.00	5.67
MOTA	2603		LEU	393	-16.579	3.772	40.580	1.00	12.28
MOTA	2604	C	LEU	393	-13.067	5.846	41.648	1.00	15.60
MOTA	2605	ō	LEU	393	-12.369	4.894	41.995	1.00	21.88
MOTA	2606	И	ILE	394	-12.566	7.022	41.278	1.00	15.30
ATOM ATOM	2607	CA	ILE	394	-11.133	7.280	41.183	1.00	13.08
ATOM	2608	CB	ILE	394	-10.856	8.709	40.595	1.00	12.22
ATOM	2609	CG2	ILE	.394	-9.353	9.003	40.512	1.00	6.65
ATOM	2610	CG1	ILE	394	-11.476	8.825	39.199	1.00	10.42
MOTA	2611	CD1	ILE	394	-11.308	10.181	38.555	1.00	13.03
ATOM	2612	C	ILE	394	-10.465	7.145	42.545	1.00	10.70
ATOM	2613	ō	ILE	394	-9.296	6.751	42.624	1.00	8.46
ATOM	2614	N	TYR	395	-11.198	7.470	43.612	1.00	13.66
MOTA	2615	CA	TYR	395	-10.652	7.377	44.966	1.00	13.63
ATOM	2616	CB	TYR	395	-11.518	8.160	45.957	1.00	15.60
ATOM	2617	CG	TYR	395	-10.902	8.313	47.328	1.00	16.11
MOTA	2618	CD1	TYR	395	-9.631	8.867	47.496	1.00	10.10
ATOM	2619	CE1		395	-9.063	8.992	48.756	1.00	17.16 21.34
MOTA	2620	CD2	TYR	395	-11.585	7.891	48.463	1.00	
ATOM	2621	CE2	TYR	395	-11.024	8.012	49.729	1.00	21.42 22.71
MOTA	2622	CZ	TYR	395	-9.767	8.559	49.871	1.00	19.28
MOTA	2623	OH	TYR	395	-9.233	8.648	51.133	1.00	13.33
ATOM	2624	C	TYR	395	-10.560	5.915	45.366	1.00	11.26
MOTA	2625	0	TYR	395	-9.488	5.432	45.741	1.00	12.67
ATOM	2626	N	LYS	396	-11.667	5.196	45.209	1.00 1.00	20.01
MOTA	2627	CA	LYS	396	-11.718	3.783	45.536	1.00	26.69
MOTA	2628	CB	LYS	396	-13.112	3.220	45.276 46.350	1.00	25.29
ATOM	2629	CG	LYS	396	-14.136	3.554		1.00	28.95
MOTA	2630	CD	LYS	396	-15.474	2.913	46.019 47.026	1.00	28.60
MOTA	2631	CE		396	-16.543	3.291	46.513	1.00	33.35
MOTA	2632	NZ	LYS	396	-17.906	2.976	44.747	1.00	22.43
MOTA	2633	C	LYS	396	-10.690	2.989 2.010	45.250	1.00	26.83
MOTA	2634	0	LYS	396	-10.143			1.00	19.52
MOTA	2635	N	GLU	397	-10.402 -9.427	3.420 2.720		1.00	18.90
MOTA	2636			397		3.106		1.00	19.12
MOTA	2637	CB	GLU	397	-9.590	2.003		1.00	18.47
MOTA	2638	CG		397	-9.221 -10.160	0.826		1.00	18.19
MOTA	2639			397	-9.669	-0.323			27.13
MOTA	2640		1 GLU	397	-11.390	1.044			14.60
MOTA	2641		2 GLU	397	-8.004	3.014			20.33
MOTA	2642		GLU	397	-7.128				22.46
ATOM	2643		GLU	397	-7.792				
MOTA	2644		VAL	398	-6.478		-		
MOTA	2645			398	-6.339				
ATOM	2646			398	-4.986				
MOTA	2647		1 VAL	398	-6.520				22.38
ATOM	2648		2 VAL	398	-6.175				
MOTA	2649		VAL		-5.001				
MOTA	2650		VAL		-7.230				
MOTA	2651		MET		-7.230			_	
MOTA	2652				-8.149				
MOTA	2653	3 CE	B MET	333	<b>2</b> · –				

## FIG. 1TT

MOTA	2654	CG	MET	399	-7.994	5.465	48.863	1.00	29.75
MOTA	2655	SD	MET	399	-6.663	5.989	50.009	1.00	40.78
MOTA	2656	CE	MET	399	-5.137	5.902	49.010	1.00	35.81
ATOM	2657	C	MET	399	-7.015	1.820	47.942	1.00	36.50
MOTA	2658	0	MET	399	-6.886	1.323	49.063	1.00	38.05
MOTA	2659	N	ASN	400	-7.108	1.092	46.829	1.00	41.19
MOTA	2660	CA	ASN	400	7.040	-0.371	46.835	1.00	41.87
MOTA	2661	CB	asn	400	-8.265	-0.971	47.538	1.00	46.04
ATOM	2662	CG	ASN	400	-9.575	-0.383	47.044	1.00	45.40
MOTA	2663		ASN	400	-10.103	-0.785	46.009	1.00	46.19
MOTA	2664		ASN	400	-10.118	0.567	47.800	1.00	45.31
ATOM	2665	C	ASN	400	-6.917	-0.953	45.422	1.00	43.13
ATOM	2666	0	ASN	400	-5.967	-0.562	44.708	1.00	38.80
ATOM	2667	C1		1001	5.651	10.641	30.742	1.00	17.40
MOTA	2668	01		1001	4.293	10.841	30.577	1.00	20.93
ATOM	2669	N1		1001	3.768	10.022	31.594	1.00	14.28
ATOM	2670	C4		1001	4.658	9.392	32.346	1.00	11.79
ATOM	2671	C5		1001	5.954	9.761	31.740	1.00 1.00	10.46 2.00
MOTA	2672	N2		1001	8.425	9.939	31.690 31.952	1.00	4.18
ATOM	2673	C7		1001	7.307	9.217 7.912	32.368	1.00	2.00
MOTA	2674		4040		7.364	7.390	32.499	1.00	2.00
ATOM	2675	C10		1001 1001	8.638 9.698	8.129	32.226	1.00	8.25
MOTA	2676 2677	N5 C18		1001	9.607	9.366	31.841	1.00	3.21
ATOM				1001	4.715	7.838	35.779	1.00	4.77
ATOM	2678	C15 C8		1001	3.449	7.244	35.771	1.00	12.75
ATOM ATOM	2679 2680	C17			2.585	7.298	34.670	1.00	12.33
ATOM	2681		4040		3.005	7.982	33.528	1.00	14.72
ATOM	2682	C13			4.278	8.594	33.526	1.00	16.11
ATOM	2683	C19		1001	5.137	8.524	34.637	1.00	13.87
ATOM	2684	C2		1001	6.629	11.300	29.783	1.00	18.40
ATOM	2685	N3		1001	10.830	10.011	31.601	1.00	4.47
ATOM	2686	C6		1001	10.987	10.898	30.601	1.00	6.40
ATOM	2687	C3		1001	12.407	11.197	30.263	1.00	6.89
ATOM	2688	04		1001	10.094	11.460	29.962	1.00	16.54
ATOM	2689	OH2		1	11.099	24.580	40.355	1.00	26.43
ATOM	2690	OH2		2	16.034	17.889	35.924	1.00	21.43
MOTA	2691	OH2	TIP3	3	6.638	2.227	44.181	1.00	32.16
ATOM	2692	OH2	TIP3	4	20.438	1.594	42.414	1.00	32.35
MOTA	2693	OH2	TIP3	5	17.397	2.019	38.588	1.00	47.80
ATOM	2694	OH2	TIP3	6	21.365	7.894	38.349	1.00	53.39
ATOM	2695	OH2	TIP3	7	-16.615	14.917	35.305	1.00	39.74
MOTA	2696	OH2	TIP3	8	-19.383	15.176	34.969	1.00	34.63
MOTA	2697	OH2	TIP3	9	-2.647	9.079	29.753	1.00	21.81
ATOM	2698	OH2	TIP3	10		8.716	29.985	1.00	22.90
MOTA	2699	OH2	TIP3	11	-13.784	2.103	42.120	1.00	35.98
ATOM	2700		TIP3	12	0.565	-3.182	34.789	1.00	43.00
MOTA	2701		TIP3	13	0.462	-2.129	37.570	1.00	31.31
MOTA	2702		TIP3	14	11.861	-5.557	22.223	1.00	35.31
ATOM	2703		TIP3			-0.706	32.084	1.00	27.78
MOTA	2704		TIP3			17.134	45.988	1.00	17.70
ATOM	2705		TIP3	17		15.635	16.157	1.00	43.57
MOTA	2706		TIP3	18	1.603	21.090	15.391	1.00	31.70
ATOM	2707		TIP3			-0.572	11.478	1.00	12.99
MOTA	2708		TIP3			11.090	10.729	1.00	35.00
ATOM	2709		TIP3			12.127	11.831	1.00	20.04
ATOM	2710		TIP3			13.923	0.070	1.00	19.05
ATOM	2711		TIP3			2.564	4.041	1.00	35.33
ATOM	2712	OH2	TIP3	24	8.047	7.521	-8.142	1.00	32.42



MOTA	2713	OHO	TIP3	25	-16.704	19.733	2.447	1.00	18.06
ATOM	2/13	UHZ	IIPS	25					
MOTA	2714	OH2	TIP3	26	-19.392	7.013	8.226	1.00	26.38
MOTA	2715	OH2	TIP3	27	-2.939	14.818	-7.342	1.00	38.07
MOTA	2716	OH2	TIP3	28	18.620	3.235	3.927	1.00	31.48
ATOM	2717	OH2	TIP3	29	19.922	-2.960	-2.057	1.00	25.96
MOTA	2718	OH2	TIP3	30	23.569	-0.799	-6.475	1.00	42.59
MOTA	2719	OH2	TIP3	31	-14.080	-0.324	3.982	1.00	11.72
MOTA	2720	OH2	TIP3	32	-1.880	-10.669	10.357	1.00	36.98
ATOM	2721	OH2	TIP3	33	-3.231	-7.645	6.430	1.00	19.85
ATOM	2722	OH2	TIP3	34	2.195	-13.454	10.124	1.00	35.78
ATOM	2723	OH2	TIP3	35	-0.645	-13.187	10.089	1.00	19.79
ATOM	2724	OH2	TIP3	36	0.013	-10.801	22.565	1.00	30.67
ATOM	2725	OH2	TIP3	37	6.286	12.972	26.252	1.00	38.52
					END				

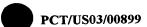
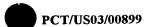


FIG. 2A

	Atom	Тур	e Res	id	<u>#</u>	x	Ā	<u>z</u>	<u>Occ</u>	<u>B</u>
ATOM	1.	N	ASP	A	45	21.903	8.714	61.519	1.00	34.40
MOTA	2	CA		A	45	21.423	9.997	62.113	1.00	36.18
MOTA	3 ·	С	ASP	Α	45	20.751	10.818	61.005~	1.00	33.68
MOTA	4	0	ASP	Α	45	19.516	10.888	60.905	1.00	33.15
MOTA	5	CB	ASP	Α	45	22.625	10.759	62.697	1.00	38.37
ATOM	6	CG	ASP	A	45	22.249	11.690	63.845	1.00	39.28
MOTA	7	OD1	ASP	Α	45	21.044	11.989	64.033	1.00	40.07
MOTA	8	OD2	ASP		45	23.181	12.121	64.563	1.00	39.46
MOTA	9	N	asn		46	21.576	11.411	60.150	1.00	31.22
ATOM	10	CA	ASN	A	46	21.053	12.210	59.046	1.00	31.07
MOTA	1.1	C	ASN		46	20.660	11.327	57.849	1.00	26.75
MOTA	12	0	ASN		46	21.383	10.407	57.490	1.00	23.97
MOTA	13	CB	ASN		46	22.087	13.258	58.623	1.00	33.86
MOTA	14	.CG	ASN		46	21.553	14.220	57.572	1.00	34.70 33.29
ATOM	15		ASN		46	20.362	14.577	57.559	1.00	34.56
MOTA	16	ND2	ASN		46	22.435	14.642	56.681	1.00 1.00	24.40
MOTA	17	N	GLN		47	19.504	11.614	57.251 56.101	1.00	23.13
MOTA	18	CA	GLN		47	18.998	10.857	54.902	1.00	20.34
ATOM	19	C	GLN		47	19.964 19.770	10.849 10.084	53.962	1.00	21.47
MOTA	20	0	GLN		47 47	17.645	11.425	55.632	1.00	26.85
MOTA	21	CB	GLN GLN		47	16.471	11.425	56.641	1.00	30.76
MOTA	22 23	CD	GLN		47	15.213	12.152	56.123	1.00	33.08
MOTA	24	ÒE1			47	14.072	11.823	56.488	1.00	27.93
ATOM ATOM	25		GLN		47	15.425	13.158	55.276	1.00	34.46
MOTA	26	NEZ	PHE		48	21.006	11.668	54.951	1.00	15.81
MOTA	27	CA	PHE		48	21.959	11.773	53.859	1.00	15.50
ATOM	28	C	PHE		48	23.318	11.257	54.197	1.00	17.92
MOTA	29	ō	PHE		48	23.602	10.946	55.343	1.00	26.00
ATOM	30	СВ	PHE		48	22.122	13.229	53.429	1.00	12.30
MOTA	31	CG	PHE	Α	48	20.835	13.880	53.069	1.00	12.37
ATOM	32		PHE	Α	48	20.014	14.361	54.047	1.00	9.42
ATOM	33	CD2	PHE	A	48	20.413	13.941	51.755	1.00	14.72
MOTA	34	CE1	PHE	Α	48	18.804	14.882	53.751	1.00	9.25
MOTA	35	CE2	PHE	Α	48	19.175	14.471	51.434	1.00	12.23
MOTA	36	CZ	PHE	Α	48	18.370	14.938	52.442	1.00	11.80
MOTA	37	N	TYR	A	49	24.158	11.165	53.177	1.00	16.03
ATOM	38	CA	TYR	Α	49	25.521	10.713	53.326	1.00	14.96
MOTA	39	C	TYR	Α	49	26.261	11.256	52.109	1.00	16.51
MOTA	40	0	TYR		49	25.634	11.623	51.120	1.00	18.27
ATOM	41	CB	TYR		49	25.579	9.179	53.444	1.00	16.48
ATOM	42	CG	TYR		49	25.594	8.371	52.160	1.00	11.73
MOTA	43		TYR		49	26.790	8.042	51.552	1.00	14.86
MOTA	44	CD2			49	24.423	7.881	51.608	1.00	10.50 16.30
ATOM	45		TYR		49	26.823	₹7.237	50.417	1.00	15.61
MOTA	46	CE2			49	24.449	7.074	50.478	1.00 1.00	16.51
ATOM	47	CZ	TYR		49	25.655	6.763	49.894 48.768	1.00	22.01
ATOM	48	ÒН	TYR		49	25.702	5.998	52.168	1.00	20.81
MOTA	49	N	SER		50 50	27.582	11.320 11.884	51.065	1.00	24.35
ATOM	50 =1	CA	SER		50 50	28.343 29.404	10.963	50.489	1.00	26.61
ATOM	51 52	C	SER SER		50	30.127	10.295	51.240	1.00	26.11
ATOM ATOM	52 53	O CB	SER		50	29.039	13.171	51.534	1.00	25.23
ATOM	53 54	OG	SER		50	28.133	14.067	52.140	1.00	26.92
MOTA	5 <del>4</del> 55	N	VAL		51	29.521	10.958	49.160	1.00	25.44
ATOM	56	CA	VAL		51	30.538	10.144	48.506	1.00	27.28

## FIG. 2B

MOTA	57	C	VAL	A	51	31.308	10.831	47.408	1.00	29.13
MOTA	58	0	VAL	A	51	30.775	11.655	46.669	1.00	28.02
MOTA	59	CB	VAL		51	30.026	8.784	47.960	1.00	25.85
ATOM	60	CG1	VAL	Α	51	30.678	7.644	48.762	1.00	23.20
MOTA	61	CG2	VAL	A	51	28.508	8.712	47.981	1.00	22.29
MOTA	62	N	GLU	Α	52	32.589	10.494	47.352	1.00	32.44
MOTA	63	CA	GLU	Α	52	33.502	11.018	46.361	1.00	37.43
MOTA	64	C	GLU	A	52	33.277	10.302	45.019	1.00	41.03
ATOM	65	0	GLU	A	52	34.044	9.393	44.658	1.00	44.17
MOTA	66	CB	GLU	A	52	34.952	10.787	46.815	1.00	40.23
MOTA	67	CG	GLU	A	52	35.354	11.489	48.122	1.00	44.49
ATOM	68	CD	GLU	A	52	36.712	11.021	48.646	1.00	45.39
ATOM	69	OE1	GLU	A	52	37.699	11.075	47.886	1.00	46.92
MOTA	70	OE2	GLU	A	52	36.792	10.577	49.814	1.00	47.73
MOTA	71	N	VAL	A	53	32.211	10.676	44.306	1.00	39.71
MOTA	72	CA	VAL	Α	53	31.918	10.099	42.992	1.00	36.87
MOTA	73	C	VAL	A	53	32.786	10.847	41.986	1.00	38.00
ATOM	74	0	VAL	A	53	32.397	11.899	41.459	1.00	36.09
MOTA	75	CB	VAL	A	53	30.435	10.252	42.576	1.00	34.18
MOTA	76	CG1	JAV	A	53	30.230	9.650	41.203	1.00	33.97
ATOM	77	CG2	VAL	A	53	29.524	9.566	43.571	1.00	28.11
ATOM	78	N	GLY	Α	54	34.005	10.349	41.806	1.00	39.05
ATOM	79	CA	GLY		54	34.931	10.956	40.871	1.00	41.22
MOTA	80	С	GLY	Α	54	35.621	12.226	41.322	1.00	42.09
MOTA	81	0	GLY	Α	54	36.625	12.185	42.036	1.00	43.69
ATOM	82	N	ASP	A	55	35.111	13.357	40.847	1.00	42.82
ATOM	83	CA	ASP	Α	55	、35.690	14.659	41.166	1.00	44.27
MOTA	84	С	ASP	A	55	34.681	15.489	41.948	1.00	43.69
MOTA	85	0	ASP	A	55	34.921	16.665	42.244	1.00	44.83
ATOM	86	CB.	ASP	A	55	36.056	15.392	39.862	1.00	44.71
ATOM	87	CG	ASP		55	37.208	16.379	40.034	1.00	45.70
MOTA	88	OD1	ASP		55	37.987	16.245	41.006	1.00	43.88
MOTA	89	OD2	ASP	A	55	37.345	17.278	39.173	1.00	45.77
ATOM	90	N	SER	A	56	33.546	14.869	42.264	1.00	41.87
MOTA	91	CA	SER		56	32.471	15.529	42.999	1.00	39.15
ATOM	92	C	SER	A	56	32.064	14.830	44.319	1.00	36.42
MOTA	93	0	SER	A	56	32.708	13.878	44.772	1.00	34.35
ATOM	94	CB	SER	Α	56	31.255	15.715	42.070	1.00	40.76
ATOM	95	OG	SER		56	30.999	14.554	41.292	1.00	44.70
MOTA	96	N	THR		57	31.060	15.397	44.977	1.00	31.87
ATOM	97	CA	THR		57	30.531	14.855	46.211	1.00	28.23
MOTA	98	C	THR		57	29.044	14.683	45.999	1.00	26.15
ATOM	99	0	THR		57	28.341	15.636	45.741	1.00	28.09
MOTA	100	CB	THR		57	30.790	15.802	47.406	1.00	25.55
ATOM	101		THR		57	32.143	15.650	47.861	1.00	22.73
MOTA	102	CG2			57	29.860	15.499	48.530	1.00	22.34
MOTA	103	N	PHE		58	28.561	13.463	46.135	1.00	26.71
MOTA	104	CA	PHE		58	27.148	13.206	45.925	1.00	27.96
MOTA	105	C	PHE		58	26.303	12.971	47.177	1.00	28.42
ATOM	106	0	PHE		58	25.740	11.892	47.379	1.00	34.14
MOTA	107	CB	PHE		58	26.963	12.040	44.960	1.00	24.54
MOTA	108	CG	PHE		58	26.701	12.457	43.533	1.00	20.20
MOTA	109		PHE		58	27.761	12.719	42.659	1.00	18.70
ATOM	110		PHE		58	25.394	12.511	43.051	1.00	17.72
MOTA	111		PHE		58	27.520	13.023	41.326	1.00	6.16
MOTA	112	CE2			58	25.143	12.816	41.716	1.00	6.65
MOTA	113	CZ	PHE		58	26.210	13.069	40.862	1.00	7.99
MOTA	114	N ~-	THR		59	26.095	14.025	47.941	1.00	26.25
ATOM	115	CA	THR	A	59	25.305	13.932	49.153	1.00	20.51



# FIG. 2C

							12 400	48.769	1.00	18.74
ATOM	116	_	THR A		59	23.921 23.123	13.489 14.273	48.293	1.00	20.15
ATOM	117	_	THR I		59	25.244	15.284	49.863	1.00	18.08
MOTA	118	_	THR I		59 59	26.585	15.707	50.146	1.00	17.42
MOTA	119		THR .		59	24.450	15.190	51.151	1.00	17.08
MOTA	120 121	CG2 N	VAL .		60	23.647	12.208	48.953	1.00	17.47
MOTA	122	CA	VAL		60	22.344	11.668	48.611	1.00	15.56
ATOM ATOM	123	C	VAL		60	21.676	10.974	49.764	1.00	9.70
MOTA	124	ō	VAL		60	22.300	10.636	50.742	1.00	11.46
ATOM	125	СВ	VAL		60	22.447	10.666	47.399	1.00	17.14
ATOM	126	CG1	·VAL	Α	60	22.985	11.395	46.174	1.00	16.49 13.46
ATOM	127	CG2	VAL	A	60	23.379	9.471	47.739	1.00	12.17
MOTA	128	N	LEU	Α	61	20.380	10.780	49.637	1.00	19.00
MOTA	129	CA	LEU		61	19.609	10.070	50.642 50.711	1.00	21.44
MOTA	130	C	LEU		61	20.217	8.665	49.680	1.00	24.40
MOTA	131	0	LEU		61	20.570	8.091 9.991	50.207	1.00	17.94
MOTA	132	CB	LEU		61	18.130	11.258	50.276	1.00	16.60
MOTA	1.33	CG	LEU		61	17.263	11.250	49.448	1.00	13.63
MOTA	134		LEU		61	16.002 16.908	11.606	51.740	1.00	16.01
MOTA	135		LEU		61	20.357	8.127	51.917	1.00	23.01
MOTA	136	N	LYS		62	20.357	6.803	52.133	1.00	21.23
MOTA	137	CA	LYS		62 62	20.420	5.611	51.334	1.00	19.20
MOTA	138	C	LYS		62	21.134	4.627	51.177	1.00	17.05
MOTA	139	0	LYS		62	20.926	6.471	53.627	1.00	22.99
MOTA	140	CB	LYS		62	22.037	7.137	54.381	1.00	21.04
ATOM	141	CG CD	LYS		62	21.743	7.287	55.857	1.00	23.25
MOTA	142 143	CE	LYS		62	22.916	8.006	56.539	1.00	23.94
ATÓM ATOM	144	NZ	LYS		62	22.712	8.217	58.005	1.00	20.22
ATOM	145	N	ARG		63	19.167	5.677	50.877	1.00	17.63
ATOM	146	CA	ARG		63	18.548	4.610	50.083	1.00	17.67
ATOM	147	C	ARG		63	19.300	4.304	48.780	1.00	20.60
ATOM	148	Ō	ARG	A	63	19.006	3.288	48.146	1.00	25.79
ATOM	149	CB	ARG	Α	63	17.097	4.968	49.745	1.00	13.35 11.45
ATOM	150	CG	ARG	Α	63	16.953	6.318	49.069	1.00	7.72
ATOM	151	CD	ARG	Α	63	15.512	6.740	48.897	1.00 1.00	6.68
ATOM	152	NE	ARG	Α	63	14.811		47.963	1.00	7.81
MOTA	153	CZ	ARG	Α	63	13.529		47.671	1.00	13.19
MOTA	154	NH:			63 ·	12.801		48.229 46.851	1.00	13.87
MOTA	155	NH:			63	12.949		48.385		21.13
MOTA	156	N	TYR		64	20.246		47.167		16.30
MOTA	157	CA			64	21.052 22.460		47.539		17.65
MOTA	158	C	TYF			23.174		48.283		19.10
ATOM	159		TYF			21.081				12.30
MOTA	160					19.691				7.10
MOTA	161					18.815				6.87
ATOM	162		1 TYF			19.235				5.16
ATOM	163		2 TYI			17.523			1.00	2.99
ATOM	164		1 TYI			17.932			1.00	3.57
MOTA	165					17.079	7.767		1.00	5.43
MOTA	166 167			RA		15.773		45.320	1.00	6.01
MOTA MOTA	168		GL			22.820		47.064		20.73
ATOM	169			N A		24.09	5 2.737			18.99
ATOM	170			N A		24.88		46.124		19.39
ATOM	173			N A		24.35	3 2.438			23.28
ATOM	172			N P		. 23.82	4 1.442			23.17
MOTA	173			N F		22.95				
MOTA	174			N A		21.66	6 0.843	49.32	1.00	33.61
				_						

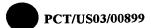
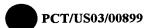


FIG. 2D

ATOM	175	OE1	GLN	Α	65	20.649	1.243	48.714	1.00	37.34
ATOM	176	NE2	GLN	A	65	21.690	-0.306	50.016	1.00	29.61
ATOM	177	N	ASN	A	66	26.155	2.131	46.303	1.00	20.73
ATOM	178	CA	ASN	Α	66	27.040	1.837	45.205	1.00	22.18
ATOM	179	С	ASN	Α	66	26.912	2.829	44.044	1.00	23.64
ATOM	180	ō	ASN		66	26.592	2.442	42.915	1.00	21.80
MOTA	181	CB	ASN		66	26.807	0.423	44.711	1.00	23.36
ATOM	182	CG	ASN		66	28.104	-0.320	44.454	1.00	23.74
ATOM	183		ASN		66	28.102	-1.548	44.360	1.00	30.68
ATOM	184	ND2	ASN		66	29.217		44.365	1.00	19.97
ATOM	185	N	LEU		67	27.195	4.105	44.329	1.00	26.13
		CA	LEU		67	27.125	5.169	43.321	1.00	26.96
MOTA	186	C	LEU		67	28.303	5.048	42.370	1.00	27.05
MOTA	187				67	29.454	4.966	42.806	1.00	23.63
MOTA	188	0	LEU			27.167	6.560	43.963	1.00	27.02
ATOM	189	CB	LEU		67 67	26.214	6.979	45.083	1.00	26.97
ATOM	190	CG	LEU		67		8.482	44.896	1.00	23.30
ATOM	191	CD1	LEU		67	25.953			1.00	22.27
ATOM	192	CD2	LEU		67	24.905	6.196	45.058	1.00	27.57
ATOM	193	N	LYS		68	28.012	5.049	41.075	1.00	27.90
ATOM	194	CA	LYS		68	29.052	4.935	40.063		
ATOM	195	С	LYS		68	28.769	6.004	39.015	1.00	26.86
ATOM	196	0	LYS		68	27.631	6.206	38.628	1.00	29.53
MOTA	197	CB	LYS		68	29.002	3.532	39.445	1.00	31.18
MOTA	198	CG	LYS	Α	68	30.135	3.254	38.466	1.00	41.51
ATOM	199	CD	LYS	Α	68	30.117	1.819	37.930	1.00	45.53
ATOM	200	CE	LYS		68	31.469	1.443	37.291	1.00	48.89
ATOM	201	NZ	LYS	Α	68	31.615	-0.040	37.036	1.00	50.37
MOTA	202	N	PRO	Α	69	29.804	6.701	38.539	1.00	27.17
ATOM	203	CA	PRO	A	69	29.622	7.756	37.532	1.00	26.52
ATOM	204	C	PRO	Α	69	29.270	7.270	36.140	1.00	25.11
ATOM	205	0	PRO	Α	69	29.877	6.336	35.617	1.00	25.86
MOTA	206	CB	PRO	Α	69	30.989	8.443	37.511	1.00	26.89
MOTA	207	CG	PRO	Α	69	31.938	7.293	37.725	1.00	28.83
ATOM	208	CD	PRO	A	69	31.231	6.524	38.863	1.00	28.51
ATOM	209	N	ILE	Α	70	28.259	7.899	35.556	1.00	24.95
ATOM	210	CA	ILE	Α	70	27.845	7.586	34.202	1.00	25.17
ATOM	211	C	ILE	A	70	27.639	8.877	33.415	1.00	26.56
ATOM	212	0	ILE	Α	70	28.656	9.620	33.256	1.00	26.71
ATOM	213	CB	ILE	Α	70	26.571	6.732	34.181	1.00	26.02
ATOM	214	CG1	ILE	Α	70	25.377	7.530	34.653	1.00	24.95
ATOM	215	CG2		Α	70	26.747	5.528	35.114	1.00	32.72
ATOM	216	CD1		Α	70	24.131	6.680	34.823	1.00	26.64
ATOM	217	N	GLY		73	29.035	15.317	33.639	1.00	45.08
ATOM	218	CA	GLY		73	28.781	16.123	32.424	1.00	45.96
MOTA	219	C	GLY		73	28.701	17.625	32.656	1.00	47.11
ATOM	220	ŏ	GLY		73	28.688	18.097	33.804	1.00	47.57
ATOM	221	N	ALA		74	28.619	18.359	31.544	1.00	46.79
ATOM	222	CA	ALA		74	28.545	19.825	31.525	1.00	45.55
	223	C	ALA		74	27.288	20.405	32.169	1.00	44.71
ATOM	223	0	ALA		74 74	27.233	21.484	32.763	1.00	44.95
ATOM						28.685	20.340	30.092	1.00	46.21
ATOM	225	CB	ALA		74 75	26.154	19.721	32.031	1.00	42.77
ATOM	226	N	GLN			24.920	20.209	32.648	1.00	42.40
ATOM	227	CA	GLN		75 75		19.391	33.880	1.00	40.14
ATOM	228	C	GLN		75 75	24.456	19.351	34.229	1.00	41.54
ATOM	229	0	GLN		75	23.268			1.00	41.18
ATOM	230	CB	GLN		75	23.819	20.353	31.596	1.00	42.08
ATOM	231	CG	GLN		75 75	23.758	19.231	30.590		44.75
MOTA	232	CD	GLN		75	22.721	18.190	30.950	1.00	46.19
ATOM	233	OE1	. GLN	A	75	23.036	17.003	31.044	1.00	40.13



## FIG. 2E

								•		
ATOM	234	NE2	GLN A	A	75	21.472	18.630	31.148	1.00	43.10
ATOM	235	N	GLY 7	A	76	25.427	18.818	34.585	1.00	36.77
MOTA	236	CA	GLY :	A	76	25.122	18.032	35.756	1.00	32.12 29.10
ATOM	237		GLY 3		76	25.867	16.726	35.649	1.00	28.74
MOTA	238	0	GLY 3		76	26.264	16.315	34.568	1.00 1.00	29.23
MOTA	239	N	ILE 3		77	26.126	16.107	36.791	1.00	26.79
MOTA	240	CA	ILE .		77	26.826	14.831	36.830	1.00	23.44
ATOM	241	С	ILE .		77	25.793	13.741	37.052	1.00	22.33
MOTA	242	0	ILE .		77	24.843	13.928	37.808	1.00	28.83
MOTA	243	CB	ILE .		77	27.894	14.797	37.949 38.246	1.00	30.10
MOTA	244	CG1	ILE .		77	28.438	16.221		1.00	23.11
MOTA	245	CG2	ILE		77	28.991	13.796	37.571 37.009	1.00	30.30
MOTA	246	CD1	ILE		77	28.853	17.081	36.335	1.00	20.94
MOTA	247	N	VAL		78	25.932	12.632		1.00	19.24
MOTA	248	CA	VAL		78	24.982	11.534	36.467 37.115	1.00	17.37
MOTA	249	C	VAL		78	25.671	10.326	36.884	1.00	14.75
ATOM	250	0	VAL		78	26.851	10.069		1.00	18.14
MOTA	251	CB	VAL		78	24.352	11.159	35.088 35.275	1.00	19.05
MOTA	252		VAL		78	23.139	10.244	34.357	1.00	19.83
ATOM	253	CG2	VAL		78	23.926	12.422	37.954	1.00	16.64
MOTA	254	N	CYS		79	24.922	9.618	38.681	1.00	16.84
MOTA	255	CA	CYS		79	25.417	8.453 7.314	38.618	1.00	14.35
MOTA	256	C	CYS		79	24.441	7.514	38.538	1.00	15.11
MOTA	257	0	CYS		79	23.231		40.166	1.00	16.44
MOTA	258	CB	CYS		79	25.643	8.780 9.176	40.188	1.00	30.72
MOTA	259	SG	CYS		79	27.336		38.571	1.00	14.50
MOTA	260	N	ALA		80	24.987	6.108	38.582	1.00	17.43
MOTA	261	CA	ALA		80	24.177	4.900 4.520	40.066	1.00	15.98
MOTA	262	C	ALA		80	24.150 25.122	4.761	40.795	1.00	16.01
MOTA	263	0	ALA		80	24.849		37.763	1.00	14.56
MOTA	264	CB	ALA		80	23.038	3.966	40.527	1.00	16.06
MOTA	265	N	ALA		81	23.036	3.573	41.920	1.00	15.59
ATOM	266	CA	ALA		81	21.836	2.609	42.147	1.00	15.48
MOTA	267	C	ALA		81	20.914	2.498	41.323	1.00	15.11
MOTA	268	0	ALA		81	22.775	4.791	42.814	1.00	12.88
ATOM	269	CB	ALA		81	21.926	1.933	43.297	1.00	18.71
ATOM	270	N	TYR		82	20.930	0.961	43.765	1.00	16.44
ATOM	271	CA	TYR		82 82	20.930	1.596	44.823	1.00	14.14
ATOM	272	C	TYR			20.013	2.140	45.800	1.00	14.37
ATOM	273	0	TYR		82	21.641	-0.273	44.354	1.00	15.08
MOTA	274	CB	TYR TYR		82· 82	20.690	-1.255	45.001	1.00	16.38
ATOM	275	CG			82	19.617	-1.782	44.288	1.00	13.31
MOTA	276	CD1				20.809	-1.592	46.352	1.00	14.38
ATOM	277	CD2	TYR TYR		82 82	18.684	-2.597	44.903	1.00	16.69
ATOM	278				82	19.867	-2.408	46.973	1.00	9.96
ATOM	279	CE2	TYR TYR			18.809	-2.891	46.253	1.00	11.01
MOTA	280	CZ	TYR		82 82	17.791	-3.550	46.886	1.00	10.41
MOTA	281	OH			83	18.713	1.517	44.623	1.00	15.81
ATOM	282	N	ASP ASP		83	17.777	2.073	45.567	1.00	15.84
MOTA	283	CA C	ASP		83	17.200	0.958	46.418	1.00	16.76
ATOM	284	0	ASP		83	16.277	0.256	46.004	1.00	13.18
MOTA	285				83	16.647	2.802	44.838	1.00	17.74
ATOM	286	CB CG	ASP ASP		83	15.647	3.428	45.786	1.00	19.13
ATOM	287		ASP		83	14.588	3.863	45.315	1.00	22.66
MOTA	288		ASP		83	15.914	3.500	46.997	1.00	23.77
ATOM	289	N	ALA		84	17.697	0.876	47.645		16.89
ATOM	290 291	CA	ALA			17.280	-0.126			14.73
ATOM		CA	ALA		84	15.804		48.879		13.83
MOTA	292	C	ALLA MARKET	. А	04	13.004				



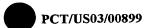
## FIG. 2F

									49.071	1.00	18.36
MOTA	293		ALA .		84		.166	-1.115	49.872	1.00	15.67
MOTA	294		ALA .		84		3.055	0.049	48.818	1.00	13.99
ATOM	295	N	VAL .	A	85		5.229	1.107		1.00	13.29
ATOM	296	CA	VAL	A	85		8.815	1.235	49.074		19.89
ATOM	297	С	VAL	A	85		2.962	0.722	47.926	1.00	24.83
MOTA	298	0	VAL	A	85	13	L.956	0.041	48.142	1.00	11.26
ATOM	299	CB	VAL	Α	85	13	3.440	2.694	49.366	1.00	
ATOM	300		VAL	A	85	1:	1.928	2.839	49.531	1.00	8.90
MOTA	301		VAL		85	14	4.186	3.165	50.597	1.00	9.72
MOTA	302	N	LEU		86	1:	3.373	1.011	46.696	1.00	22.18
ATOM	303	CA	LEU		86	1:	2.579	0.598	45.548	1.00	20.84
ATOM	304	C	LEU		86	1	3.108	-0.720	45.005	1.00	20.77
	305	o	LEU		86	1:	2.406	-1.382	44.256	1.00	24.37
MOTA	305	CB	LEU		86	1:	2.634	1.692	44.481	1.00	20.31
MOTA		CG	LEU		86		1.450	2.248	43.687	1.00	18.86
MOTA	307		LEU		86		0.348	2.823	44.545	1.00	19.36
MOTA	308		LEU		86		2.019	3.330	42.829	1.00	15.44
MOTA	309				87		4.311	-1.113	45.427	1.00	19.59
MOTA	310	N	ASP				4.952	-2.360	44.991	1.00	24.37
MOTA	311	CA	ASP		87		5.287	-2.340	43.495	1.00	27.94
ATOM	312	С	ASP		87			-3.393	42.852	1.00	30.01
ATOM	313	0	ASP		87		5.411		45.301	1.00	23.50
MOTA	314	CB	ASP		87		4.030	-3.558	45.226	1.00	20.28
MOTA	315	CG	ASP		87		4.741	-4.908	45.357	1.00	18.88
MOTA	316		ASP		87		5.985	-4.965		1.00	20.73
ATOM	317	OD2	ASP	Α	87		4.030	-5.924	45.052		27.96
ATOM	318	N	ARG	Α	88		.5.390	-1.132	42.947	1.00	24.53
ATOM	319	CA	ARG	A	88	_	5.695	-0.918	41.535	1.00	22.72
ATOM	320	. G	ARG	A	88	. 3	17.006	-0.164	41.452	1.00	21.23
ATOM	321	0	ARG	Α	88	1	L7.534	0.272	42.465	1.00	26.06
MOTA	322	CB	ARG	A	88	1	L4.601	-0.058	40.884	1.00	
ATOM	323	CG	ARG	A	88	=	L3.243	-0.708	40.833	1.00	31.50
MOTA	324	CD	ARG		88	:	12.104	0.309	40.666	1.00	37.98
MOTA	325	NE	ARG		88	:	12.189	1.086	39.426	1.00	44.46
MOTA	326	CZ	ARG		88		11.270	1.970	39.018	1.00	47.83
	327	NH:			88		10.176	2.189	39.746	1.00	46.37
MOTA	328	NH			88	:	11.452	2.659		1.00	46.81
MOTA		N	ASN		89		17.584		40.257	1.00	21.96
MOTA	329	CA	ASN		89		18.799			1.00	17.98
MOTA	330		ASN				18.171		39.394	1.00	17.64
ATOM	331	C	ASI				17.225			1.00	16.27
MOTA	332	0					19.669				21.06
MOTA	333	CB	ASI				20.241				22.14
MOTA	334		ASI				21.295				24.48
MOTA	335		1 ASI				19.564				24.86
MOTA	336		2 ASI		_		18.655	=			16.48
MOTA	337		VAI								8.72
MOTA	338	CA					18.138				7.86
MOTA	339	C	VA				19.312				6.68
MOTA	340	0	VA:	L A	90		20.446				8.10
ATOM	341	. CB		L A			17.506			_	7.17
ATOM	342	CG	1 VA	L A	90		16.307				8.82
MOTA	343		2 VA				18.555				10.32
MOTA	344			A P			19.025				14.10
MOTA	345			A A			20.064				
MOTA	346			A F			19.824	4 8.40			10.46
MOTA	347			A A			18.67	7 8.81			10.39
	348			A ?			19.91		9 36.12		11.77
MOTA				E A			20.88		7 38.97		13.28
MOTA	349			E			20.81				
MOTA	350			E			21.68				10.61
MOTA	35:	ı c	11	4							



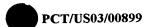
#### FIG. 2G

ATOM 352 OB ILE A 92 21.312 10.010 41.221 1.00 17.15 ATOM 353 CB ILE A 92 20.094 17.260 42.062 1.00 13.54 ATOM 355 CGZ ILE A 92 20.094 11.260 42.062 1.00 13.54 ATOM 355 CGZ ILE A 92 20.094 11.260 42.062 1.00 13.54 ATOM 355 CGZ ILE A 92 21.312 10.010 41.231 1.00 16.75 ATOM 356 CDI ILE A 92 21.240 8.459 43.256 1.00 20.93 ATOM 357 N INS A 93 21.095 12.483 38.889 1.00 14.77 ATOM 358 CA INS A 93 21.095 12.483 38.889 1.00 14.77 ATOM 360 C INS A 93 21.096 14.804 39.309 1.00 9.97 ATOM 360 O INS A 93 21.091 12.509 39.825 1.00 11.17 ATOM 361 CB INS A 93 21.091 15.280 39.825 1.00 11.17 ATOM 363 CD INS A 93 21.091 15.283 36.389 1.00 18.76 ATOM 363 CD INS A 93 21.094 15.280 39.825 1.00 12.79 ATOM 365 NZ INS A 93 21.094 15.280 39.825 1.00 22.04 ATOM 365 NZ INS A 93 21.094 15.210 34.067 1.00 22.04 ATOM 365 NZ INS A 93 21.094 15.917 35.332 1.00 22.53 ATOM 366 N INS A 94 23.154 15.298 39.533 1.00 22.04 ATOM 366 N INS A 94 23.354 15.298 39.533 1.00 10.00 ATOM 366 N INS A 94 23.354 15.298 39.533 1.00 10.00 ATOM 367 CA INS A 94 24.756 16.268 41.106 1.00 28.29 ATOM 370 CB INS A 94 24.756 16.268 41.106 1.00 9.16 ATOM 371 CG INS A 94 24.756 16.268 41.106 1.00 9.16 ATOM 373 CE INS A 94 24.756 16.268 41.106 1.00 9.16 ATOM 373 CE INS A 94 24.756 16.268 41.106 1.00 9.16 ATOM 376 CA INS A 94 24.756 16.268 41.106 1.00 9.16 ATOM 377 C LEU A 95 22.395 20.013 39.530 1.00 17.86 ATOM 378 O IEU A 95 22.395 20.013 39.530 1.00 17.86 ATOM 378 O IEU A 95 22.395 20.496 38.065 1.00 17.98 ATOM 380 CG IEU A 95 22.395 20.496 38.065 1.00 17.98 ATOM 381 CD IEU A 95 22.395 20.496 38.065 1.00 12.58 ATOM 381 CD IEU A 95 22.395 20.496 38.065 1.00 12.58 ATOM 380 CG IEU A 95 22.481 18.653 40.077 1.00 22.30 ATOM 380 CG IEU A 95 22.481 18.653 40.077 1.00 22.30 ATOM 380 CG IEU A 95 22.395 20.496 38.065 1.00 12.58 ATOM 381 CD IEU A 95 20.349 19.122 37.454 1.00 4.99 ATOM 380 CG IEU A 95 20.244 24.503 39.911 1.00 24.71 ATOM 380 CR ARG A 97 22.395 20.496 38.065 1.00 27.08 ATOM 380 CR ARG A 97 22.260 27.486 41.301 1.00 22.30 ATOM 380 CR ARG A 97 22.260 27.486 41.301 1.0			_			00	22.872	11.142	38.980	1.00	9.03
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ATOM 409 C PRE A 99 21.51 31 186 39 871 1.00 27.58										_	
ATOM 410 O PHE A 99 21.311 31.120 33.01											
	MOTA	410	, 0	PH	s ₽	3 99	21.JL	_ 51.100			



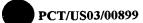
## FIG. 2H

MOTA	411	CB	PHE A			9.701	29.418	41.073	1.00 1.00	19.95 24.21
MOTA	412	CG	PHE A			0.410	28.882	42.262 42.866	1.00	25.78
MOTA	413		PHE A			9.984	27.698	42.698	1.00	23.70
MOTA	414		PHE A			1.579	29.480 27.127	43.894	1.00	26.74
MOTA	415		PHE A			0.708		43.723	1.00	27.03
MOTA	416		PHE P			2.319	28.929	44.320	1.00	26.84
MOTA	417	CZ	PHE A			1.893	27.736	39.329	1.00	20.86
MOTA	418	N	GLN I			2.790	29.411	39.203	1.00	19.24
ATOM	419	CA	GLN A			3.998	30.196 31.238	38.081	1.00	23.28
ATOM	420	C	GLN A			3.933	32.240	38.123	1.00	23.81
ATOM	421	0	GLN A			4.648	29.309	39.086	1.00	16.82
ATOM	422	CB	GLN A			5.228	28.536	37.827	1.00	16.73
MOTA	423	CG	GLN A			5.359 6.782	28.575	37.334	1.00	20.50
MOTA	424	CD	GLN A				29.215	36.325	1.00	29.92
MOTA	425	OE1				7.087	27.945	38.062	1.00	21.47
MOTA	426	NE2		A 100		7.674	30.972	37.064	1.00	23.78
MOTA	427	N		A 101		3.110	31.892	35.958	1.00	18.93
MOTA	428	CA		A 101		2.879	31.586	35.318	1.00	19.15
MOTA	429	C		A 101		1.527	30.576	35.635	1.00	16.93
MOTA	430	0		A 101		0.894		34.981	1.00	19.19
MOTA	431	CB		A 101		24.078	32.051	34.145	1.00	19.46
MOTA	432	CG		A 101		24.403	30.812 30.291	33.428	1.00	23.89
MOTA	433		ASN .			23.556		34.146	1.00	15.74
MOTA	434	ND2	ASN			25.670	30.417		1.00	21.89
MOTA	435	N		A 102		21.022	32.521	34.523	1.00	23.21
MOTA	436	CA		A 102		19.701	32.356	33.922	1.00	22.40
ATOM	437	С		A 102		19.533	31.258	32.888	1.00	21.56
ATOM	438	0		A 102		18.412	30.837	32.617	1.00	29.90
MOTA	439	CB		A 102		19.199	33.682	33.361	1.00	31.93
MOTA	440	CG		A 102		19.154	34.804	34.390		34.84
MOTA	441	CD		A 102		18.372	36.001	33.894	1.00 1.00	36.18
MOTA	442			A 102		17.132		33.899	1.00	33.10
ATOM	443	NE2		A 102		19.090		33.437 32.289	1.00	22.92
MOTA	444	N		A 103		20.634		31.312	1.00	24.22
MOTA	445	CA		A 103		20.591		32.154	1.00	23.67
MOTA	446	C		A 103		20.342		32.154	1.00	26.93
MOTA	447	0		A 103		19.277			1.00	27.86
MOTA	448	CB		A 103		21.934		30.553	1.00	24.55
MOTA	449	OGI		A 103		22.235		29.994	1.00	28.78
MOTA	450	CG2	_	A 103		21.871		29.427	1.00	25.35
MOTA	451	N		A 104		21.292		33.024		23.26
MOTA	452	CA		A 104		21.158		33.947		20.46
MOTA	453	С	HIS	A 104		19.839		34.677		24.89
MOTA	454	0		A 104		19.115		34.763	1.00	
MOTA	455	CB	HIS	A 104		22.237		35.044		23.44 22.14
MOTA	456	CG		A 104		23.612				27.61
MOTA	457	ND:	1 HIS	A 104		23.912				23.89
MOTA	458	CD	2 HIS	A 104		24.775				21.83
MOTA	459	CE	1 HIS	A 104		25.201				
MOTA	460		2 HIS	A 104		25.748				21.86
ATOM	461	N	ALA	A 105		19.506				18.99
ATOM	462			A 105		18.295	_			16.67
ATOM	463			A 105		16.977				15.43
MOTA	464			A 105		15.984				15.84
ATOM	465			A 105		18.393	1 29.746			19.42
MOTA	466			A 106		16.923				18.41
ATOM	467			A.106		15.614				20.15
MOTA	468			A 106		15.360		<b>-</b>		18.69
MOTA	469			A 106		14.232	2 26.949	32.474	1.00	20.92
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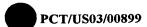
## FIG. 2I

			3 100		15.590	29.792	32.202	1.00	23.44
MOTA	470		YS A 106		14.173	30.098	31.717	1.00	27.12
MOTA	471		YS A 106		14.060	31.508	31.132	1.00	33.79
MOTA	472		LYS A 106		15.141	31.794	30.090	1.00	35.65
MOTA	473		LYS A 106		14.827	31.086	28.854	1.00	35.14
MOTA	474		LYS A 106		16.477	26.670	32.441	1.00	19.73
MOTA	475		ARG A 107		16.392	25.293	31.985	1.00	19.95
MOTA	476		ARG A 107			24.354	33.148	1.00	18.65
MOTA	477	-	ARG A 107		16.047 15.202	23.476	33.053	1.00	17.46
MOTA	478	_	ARG A 107			24.918	31.383	1.00	22.01
MOTA	479		ARG A 107		17.754 18.130	23.452	31.608	1.00	30.96
MOTA	480		ARG A 107		19.475	23.452	30.938	1.00	39.76
MOTA	481		ARG A 107			22.209	29.788	1.00	43.62
MOTA	482		ARG A 107		19.261	21.919	29.013	1.00	45.78
MOTA	483		ARG A 107		20.326	22.423	29.297	1.00	43.52
MOTA	484		ARG A 107		21.516	21.115	27.957	1.00	46.85
ATOM	485		ARG A 107		20.170	24.554	34.265	1.00	16.31
MOTA	486		ALA A 108		16.771	23.766	35.467	1.00	16.08
MOTA	487		ALA A 108		16.500		35.919	1.00	18.41
ATOM	488	C	ALA A 108		15.036	23.886		1.00	22.63
MOTA	489	0	ALA A 108		14.317	22.907	36.070	1.00	14.86
ATOM	490	CB	ALA A 108		17.430	24.262	36.580		16.47
ATOM	491	N	TYR A 109		14.616	25.143	36.183	1.00	16.30
MOTA	492	CA	TYR A 109		13.242	25.374	36.642	1.00	16.15
ATOM	493	С	TYR A 109		12.210	24.806	35.658	1.00	13.54
ATOM	494	0	TYR A 109	ı	11.180	24.267	36.041	1.00	20.39
ATOM	495	CB	TYR A 109	1	13.042	26.888	36.802	1.00	25.65
ATOM	496	CG	TYR A 109	)	11.659	27.186	37.284	1.00	25.78
ATOM	497		TYR A 109		11.298	26.891	38.598	1.00	
ATOM	498		TYR A 109		10.728	27.786	36.433	1.00	26.01
ATOM	499		TYR A 109		10.021	27.191	39.057	1.00	24.75
ATOM	500	CE2	TYR A 109		9.452	28.087	36.892	1.00	26.22
ATOM	501	CZ	TYR A 10		9.097	27.792	38.196	1.00	27.05
ATOM	502	OH	TYR A 10		7.837	28.116	38.668	1.00	28.89
ATOM	503	N	ARG A 11		12.540	24.995	34.370	1.00	17.31
ATOM	504	CA	ARG A 11		11.619	24.594	33.311	1.00	17.38
ATOM	505	C	ARG A 11		11.421	23.077	33.279	1.00	14.31
	506	ō	ARG A 11		10.316	22.554	33.158	1.00	12.85
ATOM	507	CB	ARG A 11		12.198	25.061	31.983	1.00	19.68
MOTA	508	CG	ARG A 11		11.223	24.875		1.00	21.51
MOTA	509	CD	ARG A 11		11.719	25.527	29.547	1.00	21.69
MOTA	510	NE	ARG A 11		10.778	25.285	28.454		23.64
MOTA	511		ARG A 11		10.989		27.694	1.00	25.84
MOTA	511		ARG A 11		12.011	23.397	27.947	1.00	26.19
MOTA	513		ARG A 11		10.170		26.677		29.07
ATOM			GLU A 11		12.559			1.00	16.41
ATOM	514		GLU A 11		12.480			1.00	17.69
MOTA	515		GLU A 11		11.636			1.00	16.80
MOTA	516		GLU A 11		10.875			1.00	17.49
MOTA	517		GLU A 11		13.908			1.00	20.48
MOTA	518				14.890				22.16
ATOM	519		GLU A 11		14.926			_	22.88
MOTA	520	) CD	GLU A 11		15.010				27.95
MOTA	521		L GLU A 11		14.874	=			22.77
MOTA	522		2 GLU A 11		11.83		_		19.48
MOTA	523		LEU A 1		11.076	=			17.81
MOTA	524				9.56				16.62
MOTA	525		LEU A 1		8.83				19.18
MOTA	526		LEU A 1						21.80
MOTA	52'		LEU A 1		11.46				
MOTA	528	B CG	LEU A 1	L2	12.51		5 55.02		



# FIG. 2J

ATOM	529	CD1	. LEU			1	1.898	20.35	7	40.131	1.00	25.56
MOTA	530	CD2				1	3.549	20.32	3	38.326	1.00	21.91
ATOM	531	N	VAL	A	113		9.097	22.04	7	36.280	1.00	20.17
ATOM	532	CA	VAL	Α	113		7.651	22.28	7	36.184	1.00	20.67
MOTA	533	C	VAL				7.012	21.57	3	34.990		
ATOM	534	0	VAL				5.802	21.40	6	34.909	1.00	21.37
ATOM	535	CB	VAL				7.417	23.79		36.067	1.00	22.41
ATOM	536		. VAL				7.918	24.49		37.324	1.00	25.86
ATOM	537		VAL				8.155	24.340		34.857	1.00	27.52
ATOM	538	N	LEU				7.823	21.15	5	34.025	1.00	21.23
ATOM	539	CA	LEU				7.302	20.468		32.852		
ATOM	540	C	LEU				6.944	19.040		33.187		
ATOM	541	0	LEU				5.970	18.517		32.679		
MOTA	542	CB	LEU				8.309	20.510		31.707		
ATOM	543	CG	LEU				8.123	21.779		30.910	1.00	
ATOM ATOM	544		LEU				9.019	21.789		29.697		
ATOM	545 546		LEU				6.658	21.846		30.529	1.00	
ATOM	546 547	N CA	MET				7.687	18.454		34.114	1.00	
ATOM	548	CA	MET MET				7.454	17.093		34.540	1.00	
ATOM	549	0	MET				6.331 6.521	16.986		35.580	1.00	
ATOM	550	СВ	MET				8.745	16.426		36.655	1.00	
ATOM	551	CG	MET				9.885	16.503 16.626		35.082	1.00	
ATOM	552	SD	MET				1.294	15.590		34.109 34.512	1.00	
ATOM	553	CE	MET				2.674	16.742		34.691	1.00	
ATOM	554	N	LYS				5.207	17.627		35.295	1.00	
ATOM	555	CA	LYS				4.016	17.560		36.128	1.00	
ATOM	556	C	LYS				2.825	17.626		35.157	1.00	
ATOM	557	0	LYS				1.662	17.676		35.566	1.00	
MOTA	558	CB	LYS				3.947	18.731		37.115	1.00	
ATOM	559	CG	LYS				4.682	18.522		38.427	1.00	
MOTA	560	CD	LYS				6.146	18.859		38.298	1.00	
ATOM	561	CE	LYS	A	116		6.956	18.386		39.509	1.00	
ATOM	562	NZ	LYS	A	116	(	6.576	19.050		40.806	1.00	
MOTA	563	N	CYS	Α	117	:	3.137	17.548	3	33.865	1.00	
MOTA	564	CA	CYS .	Α	117		2.141	17.640	)	32.801	1.00	
MOTA	565	C	CYS .			:	2.464	16.718	3	31.628	1.00	38.05
ATOM	566	0	CYS .	Α	117		1.953	16.893	3 .	30.509	1.00	38.49
ATOM	567	CB	CYS .			2	2.122	19.070		32.300	1.00	40.82
ATOM	568	SG	CYS .			3	3.811	19.677		32.161	1.00	
ATOM	569	N	VAL .				3.357	15.772	3	31.877	1.00	33.83
ATOM	570	CA	VAL .				3.745	14.819		30.869	1.00	29.05
ATOM	571	C	VAL .				3.762	13.424		31.467	1.00	29.19
ATOM	572	0	VAL				1.564	13.130		32.350	1.00	
ATOM	573	CB	VAL :				5.115	15.167		30.286	1.00	22.96
ATOM	574		VAL				5.005	16.461		29.515	1.00	23.45
ATOM	575		VAL 2				5.169	15.270		31.382	1.00	21.58
ATOM	576	N	THR I				2.805	12.594		31.071	1.00	28.43
ATOM	577 570	CA	THR I				2.773	11.232		31.580	1.00	26.35
ATOM ATOM	578 579	C 0	THR 2				2.964	10.272		30.401	1.00	21.80
ATOM	580	CB	THR I				2.026	9.812		29.759	1.00	17.32
ATOM	581		THR A				499	10.962		32.474	1.00	29.38
ATOM	582		THR A				657	9.720		33.177	1.00	28.88
ATOM	583	N N	HIS A				.187 .229	10.966 10.043		31.656 30.077	1.00	28.91
ATOM	584	CA	HIS A				.538	9.181		28.971	1.00	21.71
ATOM	585	C	HIS A					8.329		29.189	1.00	18.80 19.60
ATOM	586	ō	HIS A				.767	8.795		29.673	1.00	18.49
ATOM	587	CB	HIS A				.714	9.979		27.697	1.00	22.81
	-			- •		-			•			· O I



## FIG. 2K

	MOTA	588	CG	HIS 2	A 120	4.446	9.182	26.457	1.00	19.79
	ATOM	589		HIS 2			8.948	25.993	1.00	20.77
	ATOM	590		HIS 2			8.571	25.595	1.00	21.10
	MOTA	591	CE1	HIS 2	A 120	3.236	8.229	24.887	1.00	20.93
	ATOM	592	NE2	HIS A	A 120	4.507	7.984	24.623	1.00	22.50
	ATOM	593	N	LYS 2	A 121	5.632	7.093	28.702	1.00	21.55
	MOTA	594	CA	LYS 2	A 121	6.652	6.069	28.798	1.00	18.22
	ATOM	595	C	LYS 2			6.406		1.00	15.50
	ATOM	596	0	LYS 2			5.894	28.204	1.00	13.13
	ATOM	597	CB	LYS Z	A 121	6.061	4.700	28.425	1.00	23.17
	ATOM	598	CG	LYS 2	A 121		4.668	27.137	1.00	24.31
	ATOM	599	CD	LYS A			3.295	26.862	1.00	23.40
	ATOM	600	CE	LYS A			2.249	26.709	1.00	27.84
	ATOM	601	NZ	LYS A			0.856	26.420	1.00	31.61
	ATOM	602	N	ASN A			7.328	27.008	1.00	17.11
	ATOM	603	CA	ASN A			7.778	26.123	1.00	17.46
	ATOM	604	C	ASN A			9.120	26.527	1.00	17.20
	MOTA	605	0	ASN A			9.589	25.898	1.00	16.39
	ATOM	606	СВ	ASN A			7.788	24.675	1.00	15.86
	ATOM	607	CG	ASN A			6.435	24.232	1.00	12.87
	ATOM	608		ASN A		6.661	6.282	23.774	1.00	11.71
	ATOM	609	ND2				5.430	24.435	1.00	11.51
	ATOM	610	N	ILE A			9.717	27.590	1.00	18.46
	ATOM	611	CA	ILE A			10.980	28.131	1.00	20.03
	ATOM	612	C	ILE A		9.827	10.696	29.557		
	ATOM	613	Õ	ILE A		9.234	9.878	30.269	1.00	19.81 19.83
	ATOM	614	CB	ILE A			12.111	28.216		16.40
	ATOM	615		ILE A		7.667	12.431	26.837	1.00	
	ATOM	616	CG2				13.316		1.00	18.54
	ATOM	617	CD1				12.778	28.880 25.747		14.23
	ATOM	618	N	ILE A			11.382	29.982	1.00	14.50
	ATOM	619	CA	ILE A			11.194	31.320	1.00 1.00	21.80
	ATOM	620	C	ILE A			11.441	32.440	1.00	21.44 20.65
	ATOM	621	Ö	ILE A			12.360	32.384	1.00	
	ATOM	622	CB	ILE A			12.089	31.552	1.00	17.78 23.19
	ATOM	623	CG1			13.191	11.918	32.985	1.00	23.19
	ATOM	624	CG2			12.343	13.531	31.233	1.00	22.16
	ATOM	625	CD1			14.248	12.902			
	ATOM	626	N	SER A		10.479	10.549	33.409	1.00 1.00	25.57
	ATOM	627	CA	SER A		9.622	10.549	33.428 34.629	1.00	25.24
,	ATOM	628	C	SER A		10.533	10.584	•		25.57
	ATOM	629	Ö	SER A		11.474	9.799	35.852 35.943	1.00	22.29
	ATOM	630	СВ	SER A		8.734			1.00	19.83
	ATOM	631	OG	SER A		7.709	9.328	34.726 33.751	1.00	29.09
	ATOM	632		LEU A						39.45
	ATOM	633	N CA			10.225	11.425	36.819	1.00	21.25
	ATOM	634	CA	LEU A		11.059	11.458	37.995	1.00	21.80
	ATOM	635		LEU A		10.529	10.576	39.140	1.00	20.60
			0			9.315	10.470	39.376	1.00	15.37
	ATOM ATOM	636	CB	LEU A		11.276	12.907	38.418	1.00	26.09
		637	CG	LEU A		12.013	13.745	37.363	1.00	24.09
	ATOM ATOM	638		LEU A		12.074	15.165	37.840	1.00	27.50
		639		LEU A		13.421	13.246	37.149	1.00	21.86
	ATOM	640	N	LEU A		11.449	9.843	39.759	1.00	19.81
	ATOM	641	CA	LEU A		11.119	8.960	40.878	1.00	16.92
	ATOM	642	C	LEU A		11.264	9.740	42.183	1.00	17.28
	ATOM	643	0	LEU A		10.511	9.525	43.135	1.00	18.90
	ATOM	644	CB	LEU A		12.098	7.793	40.924	1.00	11.43
	ATOM	645	CG	LEU A		11.998	6.826	39.769	1.00	7.89
	ATOM	646	CDI	LEU A	127	13.068	5.751	39.875	1.00	4.22



#### FIG. 2L

MOTA	647	CD2	LEU	A	127	10	.606	6.278	3	9.816	1.00	8.16
MOTA	648	N	ASN	A	128	12	2.231	10.654	4	2.192	1.00	16.69
MOTA	649	CA	ASN	Α	128	12	.539	11.446	4	3.353	1.00	18.74
MOTA	650	С	ASN	Α	128	13	.351	12.676	4	2.968	1.00	18.70
ATOM	651	0	ASN	A	128	14	.103	12.660	4	1.991	1.00	18.08
MOTA	652	CB	ASN	A	128	13	.353	10.584	4	4.330	1.00	19.51
MOTA	653	CG	ASN	Α	128	13	3.348	11.125	4	5.753	1.00	17.80
ATOM	654	OD1	ASN	A	128	14	.249	10.836	4	6.542	1.00	17.49
MOTA	655	ND2	ASN	Α	128	12	2.307	11.863		6.100	1.00	12.82
MOTA	656	N	VAL	Α	129	13	3.135	13.748		3.732	1.00	19.15
MOTA	657	CA	VAL	Α	129		3.838	15.033		3.600	1.00	18.43
ATOM	658	C	VAL	Α	129	14	1.154	15.415		5.038	1.00	14.75
MOTA	659	0	VAL	A	129	13	3.290	15.335	4	5.902	1.00	16.11
MOTA	660	CB	VAL	A	129	12	2.923	16.178	4	3.039	1.00	17.78
MOTA	661	CG1	VAL	A	129	13	3.751	17.457		2.790	1.00	17.05
ATOM	662	CG2	VAL	Α	129	1:	2.207	15.726		1.790	1.00	17.58
MOTA	663	N	PHE	Α	130	1.9	5.367	15.830		5.321	1.00	12.66
ATOM	664	CA	PHE	Α	130	19	5.631	16.194	4	6.680	1.00	14.68
ATOM	665	C	PHE	A	130	10	5.845	17.095	4	6.773	1.00	14.31
ATOM	666	0	PHE	А	130	1'	7.567	17.283	4	5.802	1.00	14.60
ATOM	667	CB	PHE	A	130	1.9	5.835	14.914	4	7.533	1.00	11.21
MOTA	668	CG	PHE	A	130	1	7.098	14.147	4	7.199		6.13
MOTA	669	CD1	PHE	Α	130	1'	7.060	13.050	4	6.351	1.00	5.37
MOTA	670	CD2	PHE	A	130	1	3.311	14.555	4	7.690	1.00	2.00
ATOM	671	CE1	PHE	A	130	1:	3.212	12.387	4	6.016	1.00	2.00
MOTA	672	CE2	PHE	A	130	1:	9.468	13.894	4	7.358	1.00	2.88
ATOM	673	CZ	PHE	A	130	1:	9.409	12.807	4	6.506	1.00	2.00
ATOM	674	N	THR	Α	131	1	7.019	17.705	4	7.940	1.00	14.01
MOTA	675	CA	THR	Α	131	1	8.182	18.530	4	8.197	1.00	9.41
ATOM	676	C	THR	Α	131	1	8.618	18.323	4	9.616	1.00	8.55
ATOM	677	0	THR	Α	131	1	7.817	18.310	5	0.526	1.00	8.61
ATOM	678	CB	THR	A	131	1.	7.948	20.064	4	7.962	1.00	11.54
ATOM	679	OG1	THR	Α	131	1.	9.126	20.772	4	8.335	1.00	8.08
ATOM	680	CG2	THR	A	131	1.	6.781	20.604	4	8.770	1.00	5.13
MOTA	681	N	PRO	A	132	1	9.902	18.071	4	9.806	1.00	10.38
MOTA	682	CA	PRO	Α	132	2	0.434	17.872	9	1.149	1.00	13.25
MOTA	683	C	PRO	Α	132	. 2	0.595	19.173	5	1.959	1.00	17.66
MOTA	684	0	PRO	A	132	2	1.428	19.233	5	2.856	1.00	21.50
MOTA	685	CB	PRO	A	132	2	1.798	17.237	5	0.865	1.00	11.28
ATOM	686	CG	PRO	A	132	2	2.169	17.744	4	19.510	1.00	7.43
ATOM	687	CD	PRO	A	132	2	0.873	17.659	4	18.785	1.00	8.12
MOTA	688	N	GLN	Α	133	1.	9.841	20.223	5	51.642	1.00	17.79
MOTA	689	CA	GLN	A	133		9.971	21.483	5	52.373	1.00	
ATOM	690	C	GLN	A	133	1.	8.638	21.805		52.969	1.00	15.53
MOTA	691	0	GLN	Α	133	1	7.619	21.718		52.292		15.63
MOTA	692	CB	GLN	Α	133	2	0.452	22.599	. 5	51.460	1.00	15.11
MOTA	693	CG	GLN	Α	133	2	1.948	22.515	5	51.141	1.00	7.56
MOTA	694	CD	GLN	A	133	2	2.230	21.958		19.781		6.70
ATOM	695	OE1	GLN	Α	133	2	3.330	21.479	4	19.511	1.00	5.45
MOTA	696	NE2	GLN	A	133	2	1.243	22.024	. 4	18.901	1.00	6.69
ATOM	697	N	LYS	A	134	1	8.638	22.169		54.249		21.20
ATOM	698	CA	LYS	A	134		7.385	22.410		54.949		
ATOM	699	C	LYS	A	134	1	6.695	23.726		54.799		23.18
MOTA	700	0			134	1	5.473	23.792		54.976		23.37
ATOM	701	CB	LYS	A	134	1	7.472	22.008	5	56.440	1.00	25.32
MOTA	702	CG			134	1.	8.752	22.374		57.183	1.00	33.07
MOTA	703	CD			134	1	8.695	21.936	; ;	58.677	1.00	37.91
MOTA	704	CE			134	1	9.020	20.435	5 5	58.88	1.00	39.95
MOTA	705	NZ			134	1	8.837	19.935	5 (	50.304	1.00	40.52



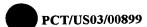
## FIG. 2M

									04 01
MOTA	706		THR A 13		17.456		54.465	1.00 1.00	24.81 22.85
MOTA	707		THR A 13		16.879	26.101	54.311 52.975	1.00	22.80
MOTA	708		THR A 1		17.225	26.694 26.415	52.431	1.00	21.61
MOTA	709		THR A 1		18.295 17.400		55.377	1.00	23.37
MOTA	710		THR A 1		18.801		55.165	1.00	21.29
ATOM	711		THR A 1: THR A 1:		17.145		56.816	1.00	23.04
MOTA	712		LEU A 1		16.357		52.506	1.00	23.87
MOTA	713 714		LEU A 1		16.553		51.240	1.00	24.40
ATOM ATOM	715	_	LEU A 1		17.903		51.250	1.00	26.61
ATOM	716		LEU A 1		18.569		50.221	1.00	30.85
ATOM	717		LEU A 1		15.436	29.283	51.002	1.00	25.03
ATOM	718	CG	LEU A 1		15.414	29.920	49.606	1.00	24.06
ATOM	719	CD1	LEU A 1	.36	13.978	30.253	49.226	1.00	24.03
MOTA	720	CD2	LEU A 1	.36	16.306		49.576	1.00	17.83
ATOM	721	N	GLU A 1	.37	18.337		52.426	1.00	25.92 25.21
ATOM	722	CA	GLU A 1		19.624		52.515	1.00	22.62
MOTA	723	С	GLU A 1		20.757	<b>-</b> -	52.378	1.00	24.90
MOTA	724	0	GLU A 1		21.843		51.969	1.00 1.00	29.36
MOTA	725	CB	GLU A 1		19.788		53.826	1.00	30.88
MOTA	726	CG	GLU A 1		18.953		53.899	1.00	33.67
MOTA	727	CD	GLU A 1		17.496		54.062 55.138	1.00	36.89
MOTA	728		GLU A 1		17.13	_	53.129	1.00	37.00
MOTA	729		GLU A 1		16.709		52.770	1.00	23.41
MOTA	730	N	GLU A		20.54		52.770	1.00	23.74
MOTA	731	CA	GLU A		21.62		51.261	1.00	20.15
MOTA	732	C	GLU A		21.70		50.825	1.00	15.33
MOTA	733	0_	GLU A		22.77		53.693	1.00	28.37
MOTA	734	CB	GLU A		21.48 21.65		55.099	1.00	34.15
MOTA	735	CG	GLU A		21.03	_	56.135	1.00	39.34
MOTA	736	CD	GLU A		19.94		56.308	1.00	41.01
MOTA	737	OE1			22.03			1.00	44.64
MOTA	738	OE2 N	PHE A		20.56	·		1.00	20.75
MOTA	739	CA	PHE A		20.36			1.00	22.38
MOTA	740 741	C	PHE A		21.47		48.215	1.00	22.59
MOTA	742	o	PHE A		21.90			1.00	22.05
MOTA	743	CB	PHE A		19.08		48.630	1.00	22.29
MOTA ATOM	744	CG	PHE A		18.68		47.353	1.00	26.18
ATOM	745		PHE A		18.79	8 24.177			27.65
ATOM	746	CD2			18.18	3 26.275	46.276		27.40
ATOM	747	CE1			18.41	.2 23.520			26.62
ATOM	748	CE2			17.78	8 25.623			27.97
ATOM	749	CZ	PHE A		17.90				24.56
ATOM	750	N	GLN A	140	21.94				23.18
MOTA	751		GLN A		22.98				20.44
ATOM	752		GLN A		22.66				19.37
ATOM	753		GLN A	140	22.60				18.41
ATOM	754		GLN A	140	24.33				15.98 23.25
MOTA	755	CG	GLN A	140	24.93				30.69
ATOM	756	CD	GLN A		26.39				35.70
MOTA	757	OE	L GLN A		. 26.83				35.70
ATOM	758	NE	2 GLN A		27.1				20.11
ATOM	759	N	ASP A	141	22.3	90 22.578			14.85
ATOM	760	CA			22.1				11.85
MOTA	761		ASP A		20.7	63 20.80			12.51
MOTA	762		ASP A		20.0	_	45.044 0 45.044		
<b>MOTA</b>	763				23.2				
MOTA	764	GG CG	ASP A	141	24.5	83 21.12	, 43.030	2 1.00	



## FIG. 2N

MOTA	765		ASP A			25.429	20.722	45.911	1.00	17.82
MOTA	766	OD2	ASP A	141	2	24.820	22.072	44.340	1.00	18.36
MOTA	767	N	VAL A			20.394	20.421	43.638	1.00	14.47
MOTA	768	CA	VAL A			L9.157	19.705	43.324	1.00	12.88
MOTA	769	C	VAL A			L9.522	18.335	42.744	1.00	13.98
MOTA	770	0	VAL A			20.330	18.222	41.807	1.00	13.92
MOTA	771	CB	VAL A			L8.319	20.492	42.321	1.00	15.25
ATOM	772	CG1	VAL A			L7.143	19.650	41.822	1.00	8.68
MOTA	773	CG2	VAL A			17.858	21.802	42.988	1.00	13.03
ATOM	774	N	TYR A			18.957	17.285	43.339	1.00	13.49 10.05
MOTA	775	CA	TYR A			19.254	15.907	42.929	1.00	8.26
MOTA	776	C	TYR A			18.036	15.312	42.298	1.00 1.00	8.82
MOTA	777	0	TYR A			16.963	15.333	42.875	1.00	5.83
MOTA	778	CB	TYR A			19.726	15.043	44.119	1.00	2.00
MOTA	779	CG	TYR A			21.153	15.323	44.558 45.400	1.00	3.10
MOTA	780	CD1				21.445	16.389	44.139	1.00	2.00
MOTA	781	CD2	TYR A			22.202	14.537	45.794	1.00	2.00
MOTA	782	CE1	TYR A			22.709	16.647	44.546	1.00	2.00
MOTA	783	CE2	TYR A			23.495	14.799 15.869	45.382	1.00	2.00
ATOM	784	CZ	TYR A			23.732	16.177	45.802	1.00	5.05
ATOM	785	OH	TYR A			25.011	14.841	41.069	1.00	12.03
MOTA	786	N	LEU A			18.202 17.091	14.260	40.328	1.00	12.86
ATOM	787	CA	LEU A			17.301	12.773	40.197	1.00	9.40
ATOM	788	C	LEU A			18.434	12.773	40.029	1.00	10.24
MOTA	789	0				16.960	14.915	38.936	1.00	12.95
ATOM	790	CB	LEU F			16.637	16.413	38.922	1.00	14.49
ATOM	791	CG	LEU F			17.061	16.992	37.585	1.00	15.65
MOTA	792		LEU F			15.152	16.691	39.211	1.00	10.66
MOTA	793 794	N N	VAL A			16.201	12.033	40.273	1.00	9.00
MOTA	794 795	CA	VAL A			16.275	10.587	40.177	1.00	7.36
MOTA MOTA	796	C	VAL A			15.288	10.023	39.164	1.00	2.00
ATOM	797	0	VAL A			14.155	10.461	39.112	1.00	2.00
ATOM	798	CB	VAL A			16.010	9.942	41.578	1.00	8.11
ATOM	799		VAL A			15.928	8.459	41.449	1.00	6.36
ATOM	800		VAL A			17.131	10.268	42.535	1.00	10.32
ATOM	801	N		A 146		15.740	9.060	38.360	1.00	6.09
ATOM	802	CA		A 146		14.891	8.380	37.351	1.00	11.90
MOTA	803	C		A 146		15.283	6.891	37.270	1.00	12.67
ATOM	804	ō	MET A			16.385	6.533	37.681	1.00	16.93
ATOM	805	СВ		A 146		15.112	8.995	35.958	1.00	13.21
ATOM	806	CG	MET I	A 146		16.477	8.650	35.322	1.00	14.34
ATOM	807	SD	MET A	A 146		16.595	9.005	33.507	1.00	17.24
ATOM	808	CE	MET I	A 146		15.195	8.091	32.828	1.00	8.30
ATOM	809	N	GLU Z	A 147		14.427	6.027	36.720	1.00	13.63
ATOM	810	CA		A 147		14.795	4.614	36.616	1.00	16.06
MOTA	811	C		A 147		16.041	4.564	35.742	1.00	16.39
MOTA	812	0	GLU 2	A 147		16.138	5.299	34.772	1.00	18.15
MOTA	813	CB	GLU	A 147		13.660	3.769	36.015	1.00	22.30
MOTA	814	CG	GLU 3	A 147	•	13.269	4.118	34.575	1.00	25.11
MOTA	815	CD		A 147		12.876	2.894	33.729	1.00	25.31
MOTA	816	OE1	GLU	A 147		13.782	2.106	33.394	1.00	30.02
MOTA	817	OE2	GLU .	A 147		11.686	2.723	33.368	1.00	23.23
MOTA	818	N		A 148		17.013	3.733	36.096	1.00	14.22
ATOM	819	CA		A 148		18.251	3.652	35.343	1.00	14.03
MOTA	820	C		A 148		18.138	3.001	33.953	1.00	19.58
MOTA	821	0		A 148		17.489	1.954	33.772	1.00	17.45
MOTA	822	CB		A 148		19.315		36.172		11.14
MOTA	823	CG	LEU	A 148		20.705	2.855	35.560	1.00	11.21



#### FIG. 20

MOTA	824	CD1	LEU A	A 148	21.451	4.189	35.640	1.00	13.69
ATOM	825		LEU A		21.464	1.797	36.305	1.00	12.65
ATOM	826	N	MET 2	A 149	18.820	3.619	32.988	1.00	18.65
MOTA	827	CA	MET A	A 149	18.820	3.148	31.618	1.00	14.79
MOTA	828	C	MET A	A 149	20.130	2.454	31.345	1.00	13.07
MOTA	829	0		A 149	21.072	2.559	32.123	1.00	11.86 14.73
MOTA	830	CB		A 149	18.658	4.327	30.640	1.00 1.00	5.61
MOTA	831	CG		A 149	17.373	5.086	30.763 30.627	1.00	10.51
MOTA	832	SD		A 149	15.962	4.060 4.372	28.976	1.00	9.66
ATOM	833	CE		A 149	15.493 20.207	1.802	30.184	1.00	14.05
MOTA	834	N		A 150 A 150	21.413	1.085	29.787	1.00	11.22
MOTA	835	CA C		A 150 A 150	22.380	1.845	28.922	1.00	10.09
MOTA	836 837	0		A 150	23.575	1.506	28.898	1.00	10.09
ATOM ATOM	838	CB		A 150	21.037	-0.230	29.130	1.00	16.26
MOTA	839	CG		A 150	20.243	-1.117	30.037	1.00	13.51
MOTA	840			A 150	20.675	-1.305	31.189	1.00	21.61
ATOM	841			A 150	19.177	-1.594	29.635	1.00	14.13
ATOM	842	N		A 151	21.892	2.860	28.203	1.00	12.49
ATOM	843	CA	ALA	A 151	22.895	3.532	27.362	1.00	11.41
ATOM	844	C	ALA	A 151	22.325	4.780	26.650	1.00	6.60
MOTA	845	0	ALA	A 151	21.144	5.071	26.685	1.00	9.62
ATOM	846	CB	ALA	A 151	23.395	2.525	26.321	1.00	15.41
ATOM	847	N		A 152	23.255	5.559	26.017	1.00	8.84
MOTA	848	CA		A 152	22.834	6.768	25.269	1.00	12.68 14.17
MOTA	849	С		A 152	22.463	6.411	23.827	1.00 1.00	12.97
ATOM	850	0		A 152	22.850	5.384 7.753	23.299 25.259	1.00	15.88
MOTA	851	CB		A 152	24.018	9.137	25.233	1.00	21.57
MOTA	852	CG		A 152	23.540 22.347	9.428	25.598	1.00	22.60
ATOM	853			A 152 A 152	24.517	10.021	25.847	1.00	22.95
ATOM	854	N NDS		A 153	21.664	7.294	23.186	1.00	15.15
ATOM ATOM	855 856	CA		A 153	21.356	7.079	21.769	1.00	15.28
ATOM	857	C		A 153	22.606	7.253	20.909	1.00	17.68
ATOM	858	Õ		A 153	22.734	6.709	19.820	1.00	21.55
MOTA	859	CB		A 153	20.278	8.089	21.339	1.00	15.66
ATOM	860	CG		A 153	19.170	7.451	20.478	1.00	17.15
ATOM	861			A 153	18.727	8.359	19.327	1.00	10.86
MOTA	862	CD2	LEU	A 153	19.602	6.127	19.840	1.00	16.75
ATOM	863	N	CYS	A 154	23.616	7.963	21.398	1.00	20.01
ATOM	864	CA	CYS	A 154	24.877	8.139	20.688	1.00	21.31
MOTA	865	C		A 154	25.586	6.786	20.532	1.00	24.69
MOTA	866	0		A 154	26.235	6.509	19.517	1.00	23.42 21.53
MOTA	867	CB		A 154	25.806	9.047	21.498	1.00	19.73
MOTA	868	SG		A 154	25.188	10.670 5.985	21.924	1.00 1.00	24.09
MOTA	869	N		A 155	25.515	4.682	21.587 21.615	1.00	22.22
MOTA	870	CA		A 155	26.140	3.715	20.676	1.00	21.75
MOTA	871	C		A 155	25.415 26.062	2.949	19.958	1.00	20.49
MOTA	872	0		A 155	26.139	4.153	23.053	1.00	22.67
ATOM	873 874	CB N		A 155 A 156	24.081	3.791	20.654	1.00	20.79
ATOM	875	CA		A 156	23.256	2.936	19.800	1.00	19.64
ATOM	876	CA		A 156	23.401	3.318	18.324	1.00	21.10
ATOM ATOM	877	Ö		A 156	23.276	2.463	17.456	1.00	22.67
MOTA	878	СВ		A 156	21.757	3.013	20.202	1.00	18.09
MOTA	879			A 156	20.898	2.256	19.209		18.46
MOTA	880	CG2		A 156	21.552	2.450	21.586		18.31
ATOM	881	N		A 157	23.665	4.597	18.046		21.10
MOTA	882	CA		A 157	23.832	5.101	16.681	1.00	21.62

FIG. 2P

ATOM	883	C	ILE A	157	25.082	4.471	16.108	1.00	21.87
MOTA	884	0	ILE A	157	25.191	4.226	14.898	1.00	20.25
MOTA	885			A 157	24.016	6.669	16.641	1.00	21.74
MOTA	886			A 157	22.662	7.363	16.670	1.00	20.08
MOTA	887	CG2	ILE 2	A 157	24.737	7.106	15.372	1.00	22.36
MOTA	888	CD1	ILE A	A 157	22.762	8.840	16.733	1.00	21.43
MOTA	889	N	GLN A	A 158	26.031	4.228	16.998	1.00	20.23
MOTA	890	CA	GLN A	A 158	27.278	3.643	16.622	1.00	19.49
MOTA	891			A 158	27.186	2.171	16.296	1.00	21.66 24.62
MOTA	892	0	GLN 2	A 158	28.176	1.580	15.856	1.00	
MOTA	893			A 158	28.276	3.816	17.732	1.00	22.75
MOTA	894			A 158	28.931	5.157	17.809	1.00	25.62
MOTA	895			A 158	30.303	5.003	18.384	1.00	28.38
MOTA	896	OE1	GLN :	A 158	31.220	4.555	17.687	1.00	29.99
MOTA	897	NE2	GLN .	A 158	30.449	5.292	19.677	1.00	29.10
MOTA	898			A 159	26.054	1.540	16.571	1.00	19.31
ATOM	899	CA	MET .	A 159	25.972	0.139	16.250	1.00	19.50
MOTA	900	С	MET .	A 159	25.159	-0.138	15.011	1.00	23.14
MOTA	901			A 159	24.439	0.720	14.505	1.00	24.42
ATOM	902			A 159	25.515	-0.695	17.439	1.00	15.90
ATOM	903			A 159	24.179	-0.404	17.999	1.00	14.14
MOTA	904	SD	MET	A 159	24.233	-0.841	19.784	1.00	23.46
MOTA	905	CE		A 159	22.592	-1.324	19.992	1.00	14.23
MOTA	906	N	GLU	A 160	25.355	-1.325	14.469	1.00	24.45
MOTA	907	CA	GLU	A 160	24.657	-1.738	13.283	1.00	25.01
MOTA	908	С		A 160	23.360	-2.398	13.709	1.00	28.90
MOTA	909	0		A 160	23.375	-3.495	14.260	1.00	32.36
MOTA	910	CB	GLU	A 160	25.531	-2.727	12.536	1.00	23.25
MOTA	911	CG	GLU	A 160	25.228	-2.838	11.093	1.00	27.17
MOTA	912	CD		A 160	26.211	-3.734	10.392	1.00	26.17
MOTA	913			A 160	26.054	-4.957	10.529	1.00	27.98 31.36
MOTA	914	OE2		A 160	27.143	-3.226	9.725	1.00	29.29
MOTA	915	N		A 161	22.240	-1.701	13.551	1.00	29.29
MOTA	916	CA		A 161	20.970	-2.295	13.937	1.00	28.20
MOTA	917	C		A 161	20.017	-2.532	12.780	1.00	29.99
MOTA	918	0		A 161	20.024	-1.820	11.769	1.00	31.73
MOTA	919	CB		A 161	20.270	-1.519	15.066	1.00	30.31
MOTA	920	CG		A 161	19.907	-0.042	15.005	1.00 1.00	29.64
MOTA	921			A 161	19.055	0.288	16.210		35.08
MOTA	922	CD2		A 161	21.170	0.803	15.010	1.00	24.93
MOTA	923	N		A 162	19.212	-3.566	12.948	1.00 1.00	24.93
MOTA	924	CA		A 162	18.233	-3.967	11.968	1.00	21.63
MOTA	925	С		A 162	17.157	-2.910	11.812	1.00	24.12
MOTA	926	0		A 162	17.296	-1.815	12.315	1.00	21.90
MOTA	927	CB		A 162	17.622	-5.284	12.401	1.00	20.75
MOTA	928	CG		A 162	17.261	-5.276	13.848	1.00	24.78
MOTA	929			A 162	16.067	-5.078	14.151	1.00	23.53
MOTA	930	OD2		A 162	18.175	-5.442	14.680	1.00	23.69
MOTA	931	Ŋ		A 163	16.106	-3.247	11.070		24.26
MOTA	932	CA		A 163	14.984	-2.340	10.815		24.23
ATOM	933	С		A 163	13.937	-2.378	11.898		25.59
MOTA	934	0		A 163	13.153	-1.435	12.051		25.62
MOTA	935	CB		A 163	14.324	-2.664	9.454		25.62
MOTA	936	CG		A 163	15.174	-2.305	8.272		24.70
MOTA	937			A 163	15.328	-1.005	7.831		28.10
MOTA	938			A 163	15.945	-3.070	7.462		24.28
MOTA	939			A 163	16.157	-0.987	6.804 6.559		26.23
MOTA	940			A 163	16.546	-2.226			25.49
MOTA	941	N	GĽŪ	A 164	13.915	-3.474	12.649	1.00	43.43



#### FIG. 2Q

	_			_ 4	12.936	-3.650	13.720	1.00	23.13
ATOM	942		GLU A 1		13.295	-2.753	14.904	1.00	15.55
ATOM	943		GLU A 1		12.427	-2.141	15.513	1.00	14.60
ATOM	944		GLU A 1			-5.124	14.129	1.00	29.26
MOTA	945		GLU A 1		12.883		12.934	1.00	37.97
ATOM	946		GLU A 1		12.827	-6.092	13.074	1.00	43.81
MOTA	947	CD	GLU A 1		13.817	-7.263		1.00	45.99
ATOM	948		GLU A		14.826	-7.294	12.326	1.00	44.01
MOTA	949	OE2	GLU A		13.589	-8.150	13.935	1.00	12.40
ATOM	950	N	ARG A	165	14.584	-2.672	15.189	1.00	15.54
MOTA	951	CA	ARG A	L65	15.110	-1.846	16.261		18.06
ATOM	952	С	ARG A		15.050	-0.355	15.857	1.00	17.13
ATOM	953	0	ARG A	165	14.479	0.488	16.556	1.00	14.64
MOTA	954	CB	ARG A	165	16.563	-2.228	16.498	1.00	18.72
MOTA	955	CG	ARG A	165	16.793	-3.685	16.735	1.00	
MOTA	956	CD	ARG A	165	16.848	-4.072	18.198	1.00	21.86
ATOM	957	NE	ARG A	165	16.861	-5.527	18.362	1.00	26.60
MOTA	958	CZ	ARG A	165	17.943	-6.293	18.269	1.00	27.31
ATOM	959	NH1	ARG A	165	19.135	-5.752	18.028	1.00	30.44
MOTA	960	NH2	ARG A	165	17.820	-7.609	18.351	1.00	27.82
ATOM	961	N	MET A	166	15.642	-0.066	14.701	1.00	18.91
MOTA	962	CA	MET A		15.702	1.257	14.121	1.00	16.85
ATOM	963	C	MET A	166	14.330	1.897	14.082	1.00	16.90
ATOM	964	ō	MET A		14.147	3.007	14.573	1.00	17.46
ATOM	965	CB	MET A		16.276	1.147	12.716	1.00	21.41
ATOM	966	CG	MET A		16.493	2.449	11.988	1.00	24.12
MOTA	967	SD	MET A		18.115	2.432	11.226	1.00	32.52
ATOM	968	CE	MET A		18.074	0.866	10.278	1.00	32.32
ATOM	969	N	SER A		13.343	1.187	13.559	1.00	14.77
ATOM	970	CA	SER A		11.996	1.716	13.487	1.00	14.86
MOTA	971	C	SER A		11.204	1.763	14.805	1.00	17.43
ATOM	972	Õ	SER A		10.276	2.576	14.917	1.00	18.84
ATOM	973	CB	SER A		11.195	0.953	12.437	1.00	18.44
ATOM	974	OG	SER A		11.017	-0.404	12.823	1.00	21.45
ATOM	975	N	TYR A		11.483		15.764	1.00	17.75
ATOM	976	CA	TYR A		10.768		17.047	1.00	14.06
ATOM	977	C	TYR A		11.286		17.785	1.00	12.00
ATOM	978	ō	TYR A		10.531	2.827	18.400	1.00	12.54
ATOM	979	СВ	TYR A		11.026	-0.410	17.879	1.00	14.32
ATOM	980	CG	TYR A		10.261	-0.453	19.200	1.00	10.40
	981		L TYR A		8.896	-0.211	19.247	1.00	14.66
MOTA MOTA	982	CD2			10.905		20.401	1.00	12.40
MOTA	983	CE			8.196	-0.201	20.467	1.00	14.22
ATOM	984	CE			10.208		21.623	1.00	6.91
	985	CZ	TYR A		8.865		21.648	1.00	11.44
MOTA	986	ОН	TYR A		8.174		22.854	1.00	15.18
MOTA	987	N	LEU A		12.586			1.00	10.99
MOTA	988	CA			13.221			1.00	13.26
MOTA	989	C	LEU A		12.63				15.32
MOTA	990	0	LEU A		12.190			1.00	14.97
MOTA	991	CB	LEU A		14.719			1.00	10.60
ATOM		CG			15.513			1.00	11.30
MOTA	992		LEU A		16.99				12.03
MOTA	993		1 LEU A		15.16				9.04
MOTA	994		LEU A		12.59				17.54
MOTA	995				12.05				17.32
MOTA	996				10.59				18.92
MOTA	997		LEU A		10.16				21.34
MOTA	998		LEU A		12.18				15.04
ATOM	999				13.43				16.49
MOTA	1000	CG	LEU A	T 10	73.43			- · - <del>-</del>	



## FIG. 2R

ATOM	1001	CD1 I	EU A	170		13.849	7.801	14.238	1.00	15.81
ATOM	1002		EU A			14.565	5.538	13.628	1.00	19.02 16.52
ATOM	1003	N T	ryr A	171		9.842	5.163	16.177	1.00	
MOTA	1004	CA T	ryr A	171		8.416	5.198	16.541	1.00	14.86 12.63
ATOM	1005		TYR A			8.178	5.805	17.964	1.00	9.35
ATOM	1006	0 7	ryr A	171		7.165	6.463	18.240	1.00	9.52
ATOM.	1007	CB 3	ryr A	171		7.853	3.760	16.462		4.84
MOTA	1008		TYR A			6.505	3.587	17.120	1.00	5.95
ATOM	1009		TYR A			5.366	4.162	16.584	1.00 1.00	6.08
ATOM	1010		TYR A			6.389	2.939	18.338	1.00	4.75
MOTA	1011		TYR A			4.153	4.109	17.246	1.00	3.46
MOTA	1012		TYR A			5.173	2.891	19.010 18.458	1.00	3.67
MOTA	1013		TYR A			4.065	3.479	19.127	1.00	8.68
MOTA	1014		TYR A			2.864	3.467	18.875	1.00	14.87
MOTA	1015		GLN A			9.099	5.503	20.249	1.00	14.72
ATOM	1016		GLN A			9.030	5.963	20.249	1.00	14.62
MOTA	1017		GLN A			9.357	7.460	21.226	1.00	12.03
ATOM	1018		GLN A			8.767	8.168	21.112	1.00	14.49
MOTA	1019		GLN A			9.956	5.107 3.735	21.412	1.00	15.16
MOTA	1020		GLN A			9.403		22.334	1.00	15.71
MOTA	1021		GLN A			10.305	2.948 2.854	23.533	1.00	13.46
MOTA	1022		GLN A			10.043	2.364	21.776	1.00	16.53
MOTA	1023		GLN A		•	11.376	7.915	19.555	1.00	16.38
MOTA	1024		MET A			10.303	9.307	19.498	1.00	16.01
MOTA	1025	CA	MET A			10.719	10.136	19.014	1.00	18.08
MOTA	1026	C	MET A			9.526 9.413	11.309	19.365	1.00	21.67
MOTA	1027	0	MET A			11.879	9.495	18.527	1.00	13.67
MOTA	1028	CB	MET F			13.172	8.828	18.907	1.00	12.28
MOTA	1029	CG	MET A			14.465	9.098	17.676	1.00	18.92
MOTA	1030	SD	MET A			15.565	7.839	17.983	1.00	11.44
ATOM	1031	CE	TEA Y			8.646	9.524	18.210	1.00	15.57
MOTA	1032	N	PEO 7			7.453	10.191	17.696	1.00	12.84
MOTA	1033	CA		A 174		6.272	10.134	18.663	1.00	14.56
MOTA	1034	C		A 174		5.423	11.013	18.649	1.00	14.93
MOTA	1035	O		A 174		7.007	9.591	16.359	1.00	15.43
MOTA	1036	CB CG		A 174		7.818	9.716	15.061	1.00	19.44
ATOM	1037		LEU :			7.204	8.752	13.999	1.00	14.81
ATOM	1038	_		A 174		7.844	11.174	14.554	1.00	14.90
ATOM	1039			A 175		6.131	9.043	19.407	1.00	14.52
MOTA	1040 1041			A 175		5.054	8.950	20.377		16.46
MOTA	1041			A 175		5.372	9.995	21.451	1.00	17.66
MOTA	1042			A 175		4.485	10.702	21.915		20.36
ATOM	1043			A 175		5.036	7.567	21.033		19.53
MOTA	1044			A 175		4.596	6.190	19.979	1.00	20.01
MOTA	1045			A 176		6.645	10.052	21.854		16.83
MOTA	1040			A 176		7.097	11.000			19.04
MOTA MOTA	1047		GLY	A 176		6.873	12.419	22.385		18.61
ATOM	1049		GLY	A 176		6.121	13.169			20.79
MOTA	1050		TLE	A 177		7.450	12.761			20.33
MOTA	1051			A 177		7.296	14.098	20.661		20.67
MOTA	1051		ILE	A 177		5.822	14.417			21.19
MOTA	1052		ILE	A 177		5.403	15.566			25.02
MOTA	1054			A 177		8.080	14.265			20.27
ATOM	1055			A 177		9.566				16.70
ATOM	1056			A 177		7.588				16.17
ATOM	105		LILE	A 177		9.865				22.15
ATOM	1058	-	LYS	A 178		5.011			1.00	20.18
ATOM	1059			A 178		3.603	13.659	19.95	3 1.00	20.86



## FIG. 2S

								_		
ATOM .	1060	С	LYS			3.021	14.122	21.278	1.00	21.67 22.72
ATOM	1061	0	LYS	A	178	2.264	15.090	21.324	1.00	
ATOM	1062	CB	LYS			2.882	12.385	19.453	1.00	22.57 23.42
MOTA	1063	CG	LYS			1.342	12.466	19.385	1.00	23.55
MOTA	1064	CD	LYS			0.831	13.317	18.231	1.00 1.00	25.60
ATOM	1065	CE	LYS			-0.664	13.641	18.369	1.00	30.22
MOTA	1066	NZ	LYS			-0.937	14.847	19.258 22.360	1.00	21.34
MOTA	1067	N	HIS			3.438	13.470	23.692	1.00	19.74
MOTA	1068	CA			179	2.928	13.780 15.203	24.066	1.00	20.78
MOTA	1069	C			179	3.300	16.017	24.469	1.00	19.29
MOTA	1070	0			179	2.459	12.803	24.714	1.00	19.07
ATOM	1071	CB			179	3.518 2.790	12.784	26.024	1.00	18.62
ATOM	1072	CG			179	1.458	12.440	26.133	1.00	19.00
MOTA	1073		HIS			3.217	13.032	27.281	1.00	16.10
MOTA	1074		HIS			1.098	12.478	27.400	1.00	16.49
MOTA	1075		HIS			2.148	12.831	28.118	1.00	16.27
MOTA	1076		HIS		180	4.574	15.498	23.882	1.00	22.10
MOTA	1077	N				5.122	16.807	24.166	1.00	22.49
ATOM	1078	CA			180 180	4.254	17.916	23.528	1.00	24.20
MOTA	1079	C			180	3.833	18.847	24.212	1.00	26.51
MOTA	1080	0			180	6.556	16.849	23.643	1.00	14.03
MOTA	1081	CB CG			180	7.665	16.998	24.674	1.00	12.96
MOTA	1082				180	7.396	16.215	25.911	1.00	14.52
ATOM	1083				180	8.981	16.643	24.071	1.00	11.14
MOTA	1084 1085	N N			181	3.888	17.745	22.258	1.00	26.53
MOTA	1085	CA			181	3.090	18.731	21.535	1.00	24.04
MOTA MOTA	1087	C			181	1.671	18.824	22.031	1.00	24.90
MOTA	1088	Ö			181	1.023	19.864	21.866	1.00	25.57
MOTA	1089	CB			181	3.057	18.398	20.046	1.00	22.90
ATOM	1090	CG			181	4.388	18.473	19.384	1.00	19.53
MOTA	1091				181	4.648	17.875	18.171	1.00	20.99
ATOM	1092				A 181	5.533	19.087	19.745	1.00	20.47
ATOM	1093				A 181	5.891	18.127	17.812	1.00	19.62
MOTA	1094				A 181	6.452	18.863	18.750	1.00	21.72
MOTA	1095	N	SE	2 2	A 182	1.176	17.745	22.634	1.00	26.36
MOTA	1096	CA	SE	2 2	A 182	-0.200	17.714	23.121	1.00	25.41 23.05
MOTA	1097	C			A 182	-0.377		24.326		23.50
MOTA	1098	0			A 182	-1.474		24.578	_	25.02
MOTA	1099	CB			A 182	-0.671		23.410		22.43
MOTA	1100	QG			A 182	0.088		24.441		25.30
MOTA	1101	N			A 183	0.730		25.026	•	23.47
MOTA	1102	CA			A 183	0.761		26.222 25.884		21.12
MOTA	1103				A 183	1.369				19.62
MOTA	1104				A 183	1.817		26.757 27.368		23.94
MOTA	1105	CB			A 183	1.541				21.16
MOTA	1106				A 184	1.393				19.99
MOTA	1107				A 184	1.906 3.398				20.18
MOTA	1108				A 184	3.924				27.13
MOTA	1109				A 184	4.092				19.83
MOTA	1110				A 185	5.534				17.77
MOTA	1111				A 185	6.106				19.73
ATOM	1112				A 185 A 185	5.691				20.08
MOTA	1113				A 185	6.044				16.71
MOTA	1114				A 185	5.433				15.07
ATOM	1115		71 TT	च्य	A 185	7.55				15.10
ATOM	1116 1117				A 185	5.470				17.54
MOTA MOTA	1118				A 186	6.983		22.573	3 1.00	20.86
ATOM	***	, 14	7.1	لندد						



#### FIG. 2T

MOTA	1119	CA	ILE	A	186	7.665	22.044	21.306	1.00	22.18
MOTA	1120	C	ILE			9.151	22.138	21.659	1.00	21.75
MOTA	1121	0	IFE			9.658	23.179	22.081	1.00	27.20
MOTA	1122	CB	ILE	Α	186	7.214	23.015	20.153	1.00	24.64
MOTA	1123		ILE			5.732	22.796	19.843	1.00	23.72
MOTA	1124		ILE			8.000	22.750	18.861	1.00	17.81
MOTA	1125		ILE			5.268	23.484	18.577	1.00	27.86
MOTA	1126	N	HIS			9.799	20.981	21.587	1.00	19.52
ATOM	1127	CA	HIS			11.207	20.786	21.931	1.00	18.54
ATOM	1128	C	HIS			12.210	21.732	21.268	1.00	18.78
MOTA	1129	0	HIS			12.834	22.542	21.932	1.00	20.80
ATOM	1130	CB	HIS			11.576	19.330	21.601	1.00	10.73
ATOM	1131	CG	HIS			12.629	18.740	22.481	1.00	3.47
MOTA	1132		HIS			13.960	19.081	22.396	1.00	6.36
MOTA	1133		HIS			12.555	17.774	23.424	1.00	2.00
MOTA	1134		HIS			14.661	18.349	23.239	1.00	2.00
MOTA	1135		HIS			13.829	17.547	23.872	1.00	2.00
ATOM	1136	N	ARG			12.411	21.534	19.968	1.00	19.66
MOTA	1137	CA	ARG			13.348	22.293	19.146	1.00	16.52
ATOM	1138	C	ARG			14.836	22.006	19.298	1.00	15.80
MOTA	1139	0	ARG			15.639	22.568	18.560	1.00	15.23
ATOM	1140	CB	ARG			13.045	23.789	19.177	1.00	14.87
ATOM	1141	CG	ARG			11.829	24.129	18.351	1.00	18.15
MOTA	1142	CD	ARG			10.890	25.057	19.053	1.00	22.53 27.78
MOTA	1143	NE	ARG			11.487	26.372	19.211	1.00	33.29
ATOM	1144	CZ	ARG			11.650	26.963	20.387	1.00	41.12
ATOM	1145		ARG			11.251	26.333	21.491	1.00 1.00	27.48
MOTA	1146	NH2	ARG ASP			12.242 15.222	28.151 21.138	20.473 20.236	1.00	15.50
MOTA	1147	N CA	ASP			16.638	20.780	20.236	1.00	13.83
MOTA MOTA	1148 1149	CA	ASP			16.861	19.314	20.692	1.00	15.26
ATOM	1150	0	ASP			17.738	18.965	21.453	1.00	16.82
ATOM	1151	СВ	ASP			17.733	21.650	21.396	1.00	14.00
MOTA	1152	CG	ASP			18.880	21.538	21.266	1.00	12.97
MOTA	1153		ASP			19.366	21.256	20.151	1.00	16.34
ATOM	1154		ASP			19.595	21.720	22.270	1.00	20.60
ATOM	1155	N	LEU			16.061	18.458	20.071	1.00	18.38
ATOM	1156	CA	LEU			16.156	17.017	20.260	1.00	17.27
MOTA	1157	C	LEU			17.489	16.511	19.704	1.00	17.59
ATOM	1158	ō	LEU			17.781	16.718	18.529	1.00	19.56
ATOM	1159	СВ	LEU			15.028	16.339	19.497	1.00	18.00
ATOM	1160	CG	LEU			14.039	15.459	20.236	1.00	19.47
MOTA	1161	CD1				13.442	14.528	19.206	1.00	24.47
ATOM	1162	CD2	LEU			14.706	14.649	21.343	1.00	17.28
ATOM	1163	N	LYS	A	191	18.316	15.907	20.550	1.00	14.84
MOTA	1164	CA	LYS			19.586	15.365	20.112	1.00	13.20
MOTA	1:165	С	LYS			19.767	13.973	20.714	1.00	15.81
MOTA	1166	0	LYS			19.235	13.671	21.772	1.00	15.29
ATOM	1167	СВ	LYS	A	191	20.744	16.280	20.480	1.00	11.69
ATOM	1168	CG	LYS	Α	191	20.654	16.909	21.812	1.00	15.09
MOTA	1169	CD	LYS	Α	191	21.862	17.810	22.036	1.00	22.46
MOTA	1170	CE	LYS	A	191	21.492	19.282	22.275	1.00	25.84
ATOM	1171	NZ	LYS			22.702	20.087	22.680	1.00	33.38
ATOM	1172	N	PRO	A	192	20.533	13.105	20.049	1.00	19.16
MOTA	1173	CA	PRO			20.703	11.735	20.539	1.00	17.61
MOTA	1174	С	PRO			21.294	11.682	21.964	1.00	14.91
MOTA	1175	0	PRO	A	192	21.023	10.783	22.747	1.00	13.47
MOTA	1176	CB	PRO	A	192	21.619	10.990	19.574	1.00	17.17
ATOM	1177	CG	PRO.	A	192	22.287	12.021	18.680	1.00	19.74

## FIG. 2U

ATOM	1178	CD	PRO .	A 192	21.274	13.253	18.799	1.00	19.71
MOTA	1179	N		A 193	22.168	12.663	22.270	1.00	14.53
MOTA	1180	CA		A 193	22.816	12.651	23.581	1.00	14.67
ATOM	1181	С		A 193	21.814	12.886	24.719	1.00	14.06
MOTA	1182	0	SER	A 193	22.076	12.622	25.884	1.00	17.22
ATOM	1183	CB		A 193	23.900	13.738	23.598	1.00	10.46
ATOM	1184	OG		A 193	23.286	15.023	23.592	1.00	15.44
ATOM	1185	N	ASN .	A 194	20.642	13.441	24.347	1.00	13.38
MOTA	1186	CA		A 194	19.607	13.678	25.352	1.00	14.45
MOTA	1187	C	ASN A	A 194	18.522	12.602	25.303	1.00	13.47
ATOM	1188	0		A 194	17.419	12.761	25.804	1.00	14.24
ATOM	1189	CB		A 194	18.994	15.055	25.096	1.00	20.06
MOTA	1190	CG		A 194	19.928	16.118	25.614	1.00	18.16
MOTA	1191	OD1	ASN I	A 194	19.977	17.242	25.116	1.00	18.33
ATOM	1192	ND2	ASN I	A 194	20.694	15.740	26.648	1.00	19.86
ATOM	1193	N	ILE A	A 195	18.864	11.489	24.626	1.00	13.73
MOTA	1194	CA	ILE 2	A 195	17.953	10.351	24.592	1.00	11.13
ATOM	1195	C	ILE A	195	18.644	9.085	25.085	1.00	10.38
ATOM	1196	0		A 195	19.810	8.829	24.817	1.00	7.75
ATOM	1197	CB		195	17.484	10.152	23.154	1.00	13.28
ATOM	1198	CG1	ILE A	A 195	16.719	11.378	22.669	1.00	13.74
ATOM	1199	CG2			16.533	8.942	23.077	1.00	10.53
ATOM	1200	CD1			16.405	11.306	21.176	1.00	15.83
ATOM	1201	N	VAL A		17.892	8.297	25.865	1.00	10.18
MOTA	1202	CA	VAL A	A 196	18.456	7.062	26.387	1.00	6.55
ATOM	1203	C	VAL A		17.579	5.860	26.027	1.00	5.22
ATOM	1204	0	VAL A	196	16.385	5.983	25.788	1.00	2.00
MOTA	1205	CB		196	18.555	7.195	27.907	1.00	3.87
MOTA	1206	CG1	VAL A		19.804	7.994	28.284	1.00	2.00
ATOM	1207	CG2			17.328	7.908	28.440	1.00	2.00
MOTA	1208	N	VAL A	197	18.236	4.710	26.026	1.00	13.84
ATOM	1209	CA	VAL A	197	17.573	3.445	25.675	1.00	15.82
MOTA	1210	C	VAL A	197	17.879	2.253	26.626	1.00	17.01
ATOM	1211	0	VAL A	197	18.991	2.119	27.152	1.00	17.00
MOTA	1212	CB	VAL A		18.008	3.045	24.251	1.00	16.24
MOTA	1213	CG1	VAL A		17.798	4.222	23.286	1.00	12.09
MOTA	1214	CG2	VAL A	197	19.488	2.637	24.266	1.00	10.94
MOTA	1215	N	LYS A	198	16.885	1.405	26.856	1.00	15.55
MOTA	1216	CA	LYS A	198	17.107	0.232	27.681	1.00	20.15
MOTA	1217	С	LYS A	198	17.396	-0.899	26.689	1.00	21.33
MOTA	1218	0	LYS A	198	16.948	-0.853	25.554	1.00	23.61
MOTA	1219	CB	LYS A	198	15.901	-0.075	28.585	1.00	21.73
MOTA	1220	CG	LYS A	198	16.229	-1.021	29.758	1.00	22.90
MOTA	1221	CD	LYS P	198	15.484	-0.642	31.034	1.00	19.80
MOTA	1222	CE	LYS A	198	14.013	-0.900	30.851	1.00	24.82
MOTA	1223	NZ	LYS A	198	13.122	-0.205	31.823	1.00	28.63
MOTA	1224	N	SER A	199	18.175	-1.888	27.110	1.00	21.24
MOTA	1225	CA	SER A	199	18.575	-3.002	26.260	1.00	21.97
ATOM	1226	C	SER A	199	17.421	-3.694	25.529	1.00	19.69
MOTA	1227	0	SER A	199	17.620	-4.306	24.490	1.00	21.65
MOTA	1228	CB	SER A	199	19.448	-4.005	27.040	1.00	24.60
ATOM	1229	OG	SER A		18.742	-4.608	28.113	1.00	28.88
MOTA	1230	N	ASP A	200	16.210	-3.541	26.045	1.00	20.67
MOTA	1231	CA	ASP A		15.024	-4.119	25.418	1.00	20.33
MOTA	1232	C	ASP A	200	14.504	-3.197	24.316	1.00	21.43
ATOM	1233	0	ASP A		13.393	-3.377	23.816	1.00	21.33
MOTA	1234	CB	ASP A	200	13.915	-4.434	26.458	1.00	22.61
MOTA	1235	CG	ASP A	200	13.503	-3.219	27.329	1.00	27.20
MOTA	1236	OD1	ASP A	200	14.060	-2.103	27.160	1.00	28.10

# FIG. 2V

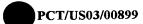
ATOM	1237		ASP			12.59	3	-3.382	28.186	1.00	26.74
ATOM	1238	N	CYS			15.31	7	-2.198	23.967	1.00	21.96
MOTA	1239	CA	CYS			15.00		-1.218	22.926	1.00	22.56
ATOM	1240	C	ĊYS			14.06	0	-0.069	23.309	1.00	22.96
MOTA	1241	0	CYS			13.80	0	0.829	22.496	1.00	22.78
ATOM	1242	CB	CYS			14.46	3	-1.936	21.689	1.00	23.72
ATOM	1243	SG	CYS			14.87		-1.138	20.161	1.00	20.78
ATOM	1244	N	THR			13.50	1	-0.117	24.516	1.00	21.58
MOTA	1245	CA	THR			12.58		0.931	24.960	1.00	18.40
ATOM	1246	C	THR			13.40		2.212	25.086		17.04
ATOM	1247	0	THR			14.63		2.158	25.289		12.40
ATOM	1248	CB	THR			11.76		0.539	26.245		21.86
MOTA	1249		THR			12.64		0.277	27.353		22.39
ATOM	1250	CG2				10.92		-0.699	25.955		17.91
ATOM	1251	N	LEU			12.73		3.352	24.882		15.72
ATOM	1252	CA	LEU			13.443		4.638	24.849		15.61
ATOM	1253	C	LEU			12.799		5.783	25.608		12.44
ATOM ATOM	1254 1255	0	LEU			11.594		5.818	25.771		14.74
ATOM	1255	CB CG	LEU LEU			13.593		5.026	23.370		13.34
ATOM	1257		LEU			14.053		6.392	22.862		13.72
ATOM	1257		LEU			14.569		6.168	21.459		13.05
ATOM	1259	N	LYS			12.885 13.603		7.421	22.904		7.57
MOTA	1260	CA	LYS			13.083		6.768 7.931	25.986		12.90
ATOM	1261	C	LYS			13.83		9.241	26.703		12.48
ATOM	1262	Ö	LYS			15.060		9.254	26.369 26.260		13.43
ATOM	1263	CB	LYS			13.149		7.676	28.215		15.08 12.82
MOTA	1264	CG	LYS			12.225		6.562	28.723		12.82
ATOM	1265	CD	LYS			12.577		6.186	30.146		16.47
ATOM	1266	CE	LYS			11.544		5.243	30.730		13.58
ATOM	1267	NZ	LYS			10.268		5.952	31.015		18.54
ATOM	1268	N	ILE			13.084		10.323	26.134	1.00	15.04
ATOM	1269	CA	ILE .			13.696		11.626	25.872		15.29
MOTA	1270	C	ILE .			13.928		12.237	27.262	1.00	14.25
MOTA	1271	0	ILE .	A 2	05	13.017	7	12.326	28.070	1.00	14.09
ATOM	1272	CB	ILE .	A 2	05	12.756	5	12.543	25.062	1.00	18.47
MOTA	1273	CG1	ILE .	A 2	05	12.417	7	11.891	23.718	1.00	19.00
ATOM	1274	CG2	ILE .	A 2	05	13.418	3	13.919	24.842	1.00	17.93
ATOM	1275	CD1	ILE A	A 2	05	11.256	5	12.571	22.962	1.00	14.77
MOTA	1276	N	LEU I	A 2	06	15.144	1	12.664	27.544	1.00	15.06
MOTA	1277	CA	LEU I	A 2	06	15.450	)	13.206	28.860	1.00	15.79
MOTA	1278	C	LEU 2			15.181	L	14.704	29.121	1.00	20.48
MOTA	1279	0	LEU A			15.034	Į.	15.108	30.287	1.00	20.24
ATOM	1280	CB	LEU A			16.898		12.901	29.201	1.00	11.74
ATOM	1281	CG	LEU A			17.372		11.468	29.137	1.00	11.09
ATOM	1282		LEU A			18.854		11.500	29.409	1.00	8.65
ATOM	1283		LEU A			16.585		10.585	30.134	1.00	7.68
MOTA	1284	N	ASP A			15.091		15.521	28.062	1.00	21.50
ATOM	1285	CA	ASP A			14.878		16.961	28.234	1.00	17.68
ATOM	1286	C	ASP A			13.672		17.490	27.490	1.00	18.35
ATOM	1287	0	ASP A			13.002		16.735	26.789	1.00	20.08
MOTA	1288	CB	ASP A			16.133		17.713	27.797	1.00	21.59
ATOM ATOM	1289 1290	CG	ASP A			16.380		17.644	26.273	1.00	29.58
ATOM	1290		ASP A			15.808		16.778	25.550	1.00	31.34
ATOM	1291		ASP A			17.184		18.471	25.799	1.00	31.59
ATOM	1293	N CA	PHE A			13.433 12.293		18.799	27.611	1.00	15.65
ATOM	1294	CA	PHE P			12.293		19.456 20.581	26.958 25.940	1.00	13.93
ATOM	1295	0	PHE A			11.741		20.381	25.523	1.00	12.22
	J	0	enn F	. 4	00	TT. /4T	•	J1/	20.523	1.00	11.22

## FIG. 2W

MOTA	1296			A 208		19.929	28.019	1.00	12.75
MOTA	1297			A 208		18.812	28.840	1.00	17.68
MOTA	1298		L PHE				30.045	1.00	19.52
ATOM	1299		PHE				28.405	1.00	18.93
ATOM	1300		L PHE			17.383	30.799	1.00	20.99
ATOM	1301		PHE .				29.145	1.00	16.66
ATOM	1302	CZ		A 208		16.704	30.349	1.00	19.20
ATOM	1303	N	GLY .				25.524	1.00	12.18
ATOM	1304	CA	GLY .			21.671	24.553	1.00	20.92
ATOM	1305	C	GLY .			23.061	25.135	1.00	26.49
ATOM	1306	0	GLY .			23.199	26.284	1.00	29.37
ATOM	1307	N	LEU .			24.094	24.355	1.00	27.55
ATOM	1308	CA	LEU .			25.481	24.814	1.00	26.38
ATOM ATOM	1309	C	LEU :			26.193	24.894	1.00	24.27
ATOM	1310	0	LEU			25.683	24.436	1.00	22.45
ATOM	1311 1312	CB CG	LEU			26.293	23.931	1.00	26.72
ATOM	1313		LEU :			25.794	22.557	1.00	22.25
ATOM	1314		LEU A			24.611	22.704	1.00	24.06
MOTA	1315	N N	ALA			25.463	21.764	1.00	
ATOM	1316	CA	ALA A			27.391	25.474	1.00	25.71
ATOM	1317	C	ALA A			28.209	25.631	1.00	25.90
ATOM	1318	ō	ALA A			28.524 28.839	24.272	1.00	27.49
ATOM	1319	CB	ALA A			29.490	24.259 26.358	1.00	30.18
ATOM	1320	·N	THR 2			33.846	24.927	1.00	28.03 39.03
ATOM	1321	CA	THR A			33.243	26.279	1.00	40.85
ATOM	1322	C	THR A			33.084	26.550	1.00	40.53
MOTA	1323	0	THR A			32.693	25.645	1.00	41.22
ATOM	1324	CB	THR A			31.869	26.349	1.00	42.09
ATOM	1325	OG1				31.013	25.325	1.00	43.36
ATOM	1326	CG2				32.032	26.133	1.00	42.14
ATOM	1327	N	PHE A			33.382	27.782	1.00	38.09
ATOM	1328	CA	PHE A	218		33.288	28.137	1.00	35.72
MOTA	1329	C	PHE A			32.253	29.213	1.00	36.31
ATOM	1330	0	PHE A	218	24.816	31.823	30.033	1.00	34.01
ATOM	1331	CB	PHE A			34.666	28.537	1.00	33.12
ATOM	1332	CG	PHE A			34.800	28.417	1.00	28.01
ATOM	1333		PHE A			35.285	29.469	1.00	23.49
ATOM	1334		PHE A			34.458	27.244	1.00	26.30
ATOM	1335		PHE A		29.397	35.418	29.364	1.00	23.12
ATOM	1336		PHE A		29.297	34.589	27.125	1.00	25.69
MOTA	1337	CZ	PHE A		30.037	35.076	28.192	1.00	24.92
MOTA	1338	N	MET A		26.913	31.875	29.184	1.00	37.55
ATOM	1339	CA	MET A		27.485	30.905	30.098		
ATOM	1340	C	MET A		29.007	31.004	30.025	1.00	35.79
ATOM	1341	0	MET A		29.556	31.607	29.105	1.00	33.20
ATOM	1342	CB	MET A		27.068	29.491	29.673	1.00	41.36
ATOM	1343	CG	MET A		25.906	28.887	30.439	1.00	44.77
ATOM	1344	SD CE	MET A		26.233	27.124	30.636	1.00	50.51
MOTA	1345		MET A		24.764	26.343	29.870	1.00	48.78
ATOM ATOM	1346 1347	N CA	MET A		29.679	30.412	31.006	1.00	38.17
ATOM	1347	CA	MET A		31.138	30.400	31.048	1.00	40.05
ATOM	1349	0	MET A		31.621	28.954	30.873	1.00	42.28
ATOM	1350	СВ	MET A		32.507	28.471	31.587	1.00	40.47
ATOM	1351	CG	MET A		31.651 31.507	31.017 32.545	32.357 32.443	1.00	40.79
ATOM	1352	SD	MET A		32.795	32.545	32.443	1.00 1.00	34.52
ATOM	1353	CE	MET A		33.047	34.823	32.693	1.00	36.04
ATOM	1354	N	THR A		31.059	28.309	29.853	1.00	36.91
<del>-</del>			·· A		32.039	20.505		T.00	45.09

FIG. 2X

MOTA	1355	CA			221		31.345	5	26.924	29	.501	1.	00	47	.82
ATOM	1356	С			221		32.628	}	26.629	28	.710	1.	00	48	.65
ATOM	1357	0			221		33.056		27.421	27	.855	1.0	00	46	.82
MOTA	1358	CB			221		30.188	3	26.313	28	.685	1.0	00	48	.78
ATOM	1359	OG1	. THR				30.476	5	24.938	28	.415	1.0	00	50	.50
MOTA	1360	CG2			221	;	30.014	Ŀ	27.066	27	.349	1.0	00	47	.96
ATOM	1361	N			222	:	33.262	?	25.480	29	.019	1.0	00	50	.08
MOTA	1362	CA	PRO	Α	222	;	34.496	;	24.999	28	.379	1.0	00	49	.33
MOTA	1363	C	PRO	A	222	:	34.168	}	24.251	27	.066	1.0	00	49	.92
MOTA	1364	0	PRO	A	222	:	35.051		24.019	26	.210	1.0	00	49	.18
ATOM	1365	CB	PRO	Α	222	;	35.078		24.038	29	.437	1.0	00	49	.23
ATOM	1366	CG			222	;	34.485	;	24.523	30	.752	1.0	00	46	.35
ATOM	1367	CD	PRO	Α	222	:	33.064	: :	24.795	30	.320	1.0	00	49	.40
MOTA	1368	N			223	;	32.896		23.879	26	.917	1.0	00	48	.31
MOTA	1369	CA	TYR	Α	223	:	32.430		23.153	25	.734	1.0	00	46	. 87
MOTA	1370	C	TYR	Α	223	:	30.998	:	23.481	25	.293	1.0	00	45	.04
ATOM	1371	0	TYR	A	223	:	30.047	٠ :	23.432	26	.080	1.0	00	42	.04
MOTA	1372	CB	TYR	A	223	;	32.605	:	21.636	25	.916	1.0	00	49	.32
ATOM	1373	CG	TYR	A	223	:	32.831	. :	21.187	27	.343	1.0	00	50	. 28
ATOM	1374	CD1	TYR			3	34.108	:	20.822	27	.784	1.0	00	49	. 70
MOTA	1375	CD2	TYR	Α	223	:	31.769	. :	21.108	28	.241	1.0	00	51	.00
ATOM	1376	CE1	TYR	Α	223	3	34.322	:	20.394	29	.088	1.0	00		.13
MOTA	1377	CE2	TYR	Α	223	3	31.973	:	20.677	29	.546	1.0	00	53	.18
MOTA	1378	CZ	$\mathbf{T}\mathbf{Y}\mathbf{R}$	Α	223	3	33.251	:	20.325	29	.961	1.0	00	53	.33
MOTA	1379	OH			223	3	33.447	:	19.933	31	.262	1.0	00	54	. 87
ATOM	1380	N	VAL			3	30.882	:	23.786	24	.002	1.0	00	44.	41
MOTA	1381	CA			224	2	29.635		24.157	23	.321	1.0	00	42	. 98
MOTA	1382	С	VAL			2	28.495	:	23.131	23	.349	1.0	00	41.	.44
MOTA	1383	0	VAL				28.700		21.949		.629	1.0	00	43.	. 91
ATOM	1384	CB	VAL				29.915		24.441		.804	1.0		42.	.37
ATOM	1385		VAL				30.677		25.739		.615			38.	
ATOM	1386	CG2					30.709		23.281		.212	1.0		41.	
ATOM	1387	N	VAL				27.292		23.596		.025	1.0		38.	
ATOM	1388	CA	VAL				26.127		22.725		.943	1.0		36.	
ATOM	1389	C	VAL				26.143		22.062		.549	1.0		35.	
ATOM	1390	0	VAL				26.917		22.446		.678	1.0		37.	
ATOM	1391	CB	VAL				24.808		23.519		.095	1.0		34.	
ATOM	1392		VAL				24.687		24.060		.485	1.0		35.	
ATOM	1393		VAL				24.755		24.650		.095	1.0		32.	
ATOM ATOM	1394	N	THR				25.302		21.061		.341	1.0		34.	
ATOM	1395 1396	CA C	THR				25.249		20.390		.051	1.0		30.	
ATOM	1397	0	THR THR				24.110		21.025		.276	1.0		27.	
ATOM	1398	CB					22.986		21.086		.767 .233	1.0		28.	
ATOM	1399		THR THR				24.978		8.896			1.0		31.	. –
ATOM	1400						86.066		.8.305		.955	1.0		34.	
ATOM	1401		THR ARG				4.793		.8.203		.893	1.0		32.	
ATOM	1402	N CA	ARG				4.394		1.484 2.135		.062	1.0		25.	
ATOM	1403	C	ARG				13.378 13.056				. 243	1.0		22.	
ATOM	1404	0	ARG				2.197		1.467		.895	1.0		20.	
ATOM	1405	CB	ARG				3.785		3.589		.163	1.0		17.	
ATOM	1406	CG	ARG				5.284		3.761		.021 .796	1.0		23.	
ATOM	1407	CD	ARG				5.649		5.158		. 294			29.	
ATOM	1407	NE	ARG				6.951		5.581		797	1.0		31.	
ATOM	1409	CZ	ARG .				7.110		6.308		898	1.0		32. 34.	
ATOM	1410		ARG .				6.044		6.693		591	1.0		34.	
ATOM	1411		ARG .				8.330		6.592		346	1.0		35.	
ATOM	1412	N	TYR .				3.678		0.320		625	1.0		20.	
ATOM	1413	CA	TYR .				3.505		9.574		359	1.0		15.	
			<b></b> .			_							-		



## FIG. 2Y

ATOM	1414	С	TYR	Α	228	22.097	19.099	14.023	1.00	14.11
MOTA	1415	0	TYR	Α	228	21.764	18.866	12.848	1.00	10.68
ATOM	1416	CB	TYR	Α	228	24.418	18.355	14.376	1.00	12.40
ATOM	1417	CG	TYR	Α	228	25.780	18.697	14.827	1.00	11.72
MOTA	1418	CD1	TYR	Α	228	26.455	17.908	15.734	1.00	16.45
MOTA	1419	CD2	TYR	Α	228	26.403	19.830	14.351	1.00	16.21
ATOM	1420	CE1				27.717	18.241	16.155	1.00	17.57
ATOM	1421	CE2	TYR	Α	228	27.661	20.177	14.761	1.00	20.39
ATOM	1422	CZ			228	28.321	19.384	15.663	1.00	18.76
ATOM	1423	ОН			228	29.585	19.751	16.061	1.00	21.49
ATOM	1424	N			229	21.272	18.977	15.058	1.00	11.87
ATOM	1425	CA	TYR			19.911	18.450	14.918	1.00	7.71
ATOM	1426	C	TYR			18.831	19.492	14.854	1.00	6.14
ATOM	1427	ō			229	17.652	19.167	14.735	1.00	7.31
ATOM	1428	CB			229	19.660	17.434	16.048	1.00	5.39
ATOM	1429	CG	TYR			20.809	16.455	16.151	1.00	2.00
ATOM	1430		TYR			21.961	16.799	16.835	1.00	
ATOM	1431	CD1				20.810	15.252			2.00
			TYR					15.434	1.00	2.00
MOTA	1432	CE1				23.089	16.004	16.800	1.00	6.24
MOTA	1433	CE2	TYR			21.957	14.428	15.399	1.00	2.47
ATOM	1434	CZ	TYR			23.091	14.813	16.080	1.00	6.64
ATOM	1435	OH	TYR			24.253	14.055	16.090	1.00	9.24
MOTA	1436	N	ARG			19.253	20.751	14.831	1.00	7.71
ATOM	1437	CA	ARG			18.322	21.869	14.789	1.00	9.82
ATOM	1438	C	ARG			17.800	22.111	13.373	1.00	7.41
MOTA	1439	0	ARG			18.558	22.066	12.417	1.00	9.37
MOTA	1440	CB	ARG			18.991	23.119	15.368	1.00	11.31
MOTA	1441	CG	ARG			19.147	23.045	16.877	1.00	13.87
MOTA	1442	CD	ARG			20.032	24.125	17.445	1.00	18.40
ATOM	1443	NE	ARG			19.874	24.196	18.899	1.00	19.51
ATOM	1444	$\mathbf{cz}$	ARG	Α	230	20.665	24.879	19.725	1.00	18.86
MOTA	1445	NH1	ARG	Α	230	21.703	25,583	19.272	1.00	22.89
MOTA	1446	NH2	ARG	A	230	20.436	24.827	21.024	1.00	14.81
ATOM	1447	N	ALA	Α	231	16.501	22.379	13.286	1.00	6.42
ATOM	1448	CA	ALA	Α	231	15.803	22.613	12.046	1.00	10.20
ATOM	1449	C	ALA	Α	231	16.222	23.941	11.442	1.00	17.23
ATOM	1450	0	ALA	Α	231	16.794	24.784	12.138	1.00	22.34
ATOM	1451	CB	ALA	Α	231	14.336	22.607	12.290	1.00	4.17
ATOM	1452	N	PRO	A	232	15.987	24.141	10.126	1.00	18.56
ATOM	1453	CA	PRO	Α	232	16.349	25.392	9.446	1.00	17.77
ATOM	1454	C.	PRO	A	232	15.590	26.590	10.010	1.00	16.05
ATOM	1455	0	PRO			16.117	27.689	10.069	1.00	14.76
ATOM	1456	СВ	PRO			15.992	25.094	7.994	1.00	18.18
ATOM	1457	CG	PRO			16.259	23.599	7.902	1.00	17.27
ATOM	1458	CD	PRO			15.575	23.130	9.142	1.00	16.24
ATOM	1459	N	GLU			14.364	26.347	10.457	1.00	16.97
ATOM	1460	CA	GLU			13.523	27.366	11.068	1.00	18.57
ATOM	1461	C	GLU			14.315	27.897	12.248	1.00	21.78
ATOM	1462		GLU			14.164	29.041	12.663	1.00	20.00
ATOM	1463	СВ	GLU			12.264	26.735	11.674	1.00	20.90
ATOM	1464	CG	GLU			11.251	26.109	10.711	1.00	22.80
ATOM	1465	CD	GLU			11.251	24.582	10.711	1.00	16.28
ATOM	1466		GLU			12.276	23.999	10.381	1.00	16.20
ATOM	1467	OE1	GLU			10.223	23.969	11.102	1.00	16.64
ATOM	1468		VAL			15.125	27.008	12.824	1.00	22.90
ATOM	1469	N					27.008	13.987	1.00	
ATOM	1470	CA	VAL VAL			15.929 17.315	27.326	13.599	1.00	18.86 20.44
MOTA	1471	C					28.788	14.179	1.00	
ATOM			VAL			17.802				23.91
WION	1472	CB	VAL	A	434	16.029	26.091	14.953	1.00	15.02

## FIG. 2Z

MOTA	1473	CG1	VAL	Α	234	17.058	26.342	16.042	1.00	12.77
MOTA	1474	CG2	VAL	A	234	14.655	25.740	15.535	1.00	7.69
MOTA	1475	N	ILE	A	235	17.942	27.197	12.604	1.00	21.11
ATOM	1476	CA	ILE	Α	235	19.272	27.633	12.183	1.00	22.08
MOTA	1477	C	ILE	Α	235	19.196	29.001	11.519	1.00	20.93
MOTA	1478	0	ILE	A	235	20.153	29.755	11.543	1.00	20.86
MOTA	1479	CB	ILE	Α	235	19.907	26.676	11.153	1.00	22.94
ATOM	1480	CG1	ILE	A	235	20.131	25.300	11.766	1.00	25.93
ATOM	1481	CG2	ILE	A	235	21.231	27.237	10.634	1.00	21.62
MOTA	1482	CD1	ILE	A	235	20.584	24.253	10.739	1.00	27.78
MOTA	1483	N	LEU	A	236	18.038	29.324	10.963	1.00	22.79
MOTA	1484	CA	LEU	A	236	17.861	30.578	10.236	1.00	24.54
ATOM	1485	C	LEU	A	236	16.960	31.601	10.911	1.00	25.47
MOTA	1486	0	LEU	Α	236	16.815	32.720	10.442	1.00	26.22
MOTA	1487	CB	LEU	A	236	17.346	30.288	8.822	1.00	21.25
ATOM	1488	CG	LEU	Α	236	18.229	29.497	7.860	1.00	16.01
MOTA	1489	CD1	LEU	A	236	17.449	29.276	6.594	1.00	13.14
ATOM	1490	CD2	LEU	A	236	19.524	30.222	7.583	1.00	10.90
MOTA	1491	N	GLY	A	237	16.315	31.198	11.987	1.00	27.03
MOTA	1492	CA	GLY	A	237	15.474	32.124	12.691	1.00	25.56
MOTA	1493	C	GLY	A	237	14.283	32.531	11.869	1.00	29.33
MOTA	1494	0	GLY	A	237	14.386	33.402	10.993	1.00	33.24
MOTA	1495	N	MET	A	238	13.184	31.808	12.070	1.00	24.71
MOTA	1496	CA	MET	Α	238	11.924	32.095	11.417	1.00	23.68
MOTA	1497	C	MET	A	238	10.871	31.472	12.289	1.00	22.36
ATOM	1498	0	MET			11.155	31.078	13.422	1.00	25.57
ATOM	1499	CB	MET	Α	238	11.876	31.559	9.980	1.00	24.38
MOTA	1500	CG	MET	Α	238	11.982	30.099	9.845	1.00	25.41
MOTA	1501	SD	MET	A	238	12.673	29.699	8.252	1.00	26.30
MOTA	1502	CE	MET	A	238	14.271	29.479	8.685	1.00	25.04
ATOM	1503	N	GLY	A	239	9.638	31.433	11.815	1.00	24.46
MOTA	1504	CA	GLY	A	239	8.589	30.833	12.621	1.00	24.89
MOTA	1505	С	GLY	A	239	8.709	29.320	12.620	1.00	25.61
MOTA	1506	0	GLY	Α	239	9.503	28.756	11.863	1.00	22.94
MOTA	1507	N	TYR	A	240	7.930	28.666	13.481	1.00	27.47
ATOM	1508	CA	TYR	A	240	7.944	27.213	13.569	1.00	26.10
MOTA	1509	C	TYR	A	240	6.608	26.662	14.028	1.00	26.67
MOTA	1510	0	TYR	A	240	5.804	27.373	14.650	1.00	<b>27.</b> 55
MOTA	1511	CB	TYR	A	240	9.070	26.715	14.514	1.00	27.69`
MOTA	1512	CG	TYR	A	240	8.888	27.004	16.000	1.00	24.07
ATOM	1513	CD1	TYR	A	240	7.908	26.360	16.736	1.00	21.50
MOTA	1514	CD2	TYR	A	240	9.666	27.973	16.650	1.00	24.16
MOTA	1515	CE1	TYR	A	240	7.688	26.673	18.083	1.00	26.09
MOTA	1516	CE2	TYR			9.453	28.300	17.995	1.00	23.28
ATOM	1517	CZ	TYR	Α	240	8.454	27.645	18.703	1.00	26.50
MOTA	1518	OH	TYR	A	240	8.158	27.979	20.006	1.00	24.58
ATOM	1519	N	LYS	Α	241	6.377	25.396	13.680	1.00	24.48
MOTA	1520	CA	LYS	Α	241	5.194	24.662	14.082	1.00	22.48
MOTA	1521	C	LYS	Α	241	5.682	23.335	14.673	1.00	21.15
ATOM	1522	0	LYS	Α	241	6.874	23.130	14.902	1.00	19.54
MOTA	1523	CB			241	4.222	24.448	12.920	1.00	23.83
MOTA	1524	CG			241	4.858	23.957	11.627	1.00	29.40
MOTA	1525	CD	LYS	Α	241	3.786	23.829	10.535	1.00	32.26
ATOM	1526	CE	LYS	A	241	4.387	23.628	9.150	1.00	31.23
MOTA	1527	NZ			241	3.361	23.218	8.134	1.00	31.87
MOTA	1528	N	GLU	Α	242	4.755	22.442	14.939	1.00	21.53
MOTA	1529	CA	GLU	Α	242	5.078	21.173	15.531	1.00	22.17
MOTA	1530	C			242	6.051	20.289	14.741	1.00	22.70
ATOM	1531	0	GLU	A	242 ,	6.770	19.486	15.340	1.00	22.12



## FIG. 2AA

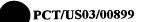
						20.433	15.830	1.00	27.33
MOTA	1532	CB	GLU A		3.780	20.433	17.004	1.00	31.09
ATOM	1533	CG	GLU A		2.964	22.345	16.700	1.00	29.61
MOTA	1534	CD	GLU A		2.268	23.358	16.428	1.00	31.84
MOTA	1535		GLU A		2.950	22.375	16.797	1.00	30.30
MOTA	1536		GLU A		1.027	20.447	13.420	1.00	20.30
MOTA	1537	N	ASN A		6.117	19.607	12.638	1.00	17.12
MOTA	1538	CA	ASN A		7.026	20.066	12.598	1.00	15.56
MOTA	1539	C	ASN A		8.465	19.540	11.835	1.00	13.73
MOTA	1540	0	ASN A		9.279	19.286	11.239	1.00	20.39
MOTA	1541	CB	ASN A		6.481	20.479	10.310	1.00	24.62
MOTA	1542	CG	ASN A		6.467	21.609	10.706	1.00	26.15
MOTA	1543		ASN A		6.777	20.227	9.045	1.00	20.34
MOTA	1544	ND2			6.116	21.022	13.457	1.00	15.14
MOTA	1545	N	VAL A		8.799	21.022	13.565	1.00	14.03
ATOM	1546	CA	VAL A		10.181	20.365	14.182	1.00	15.20
MOTA	1547	C	VAL A		11.041		13.938	1.00	17.55
MOTA	1548	0	VAL A		12.250	20.263	14.468	1.00	10.37
ATOM	1549	CB	VAL A		10.282	22.752	15.827	1.00	8.35
ATOM	1550	CG1	VAL A	244	9.645	22.489	14.615	1.00	10.44
MOTA	1551	CG2	VAL A		11.723	23.180	14.013	1.00	15.01
MOTA	1552	N	ASP F		10.396	19.513	15.637	1.00	12.69
MOTA	1553	CA	ASP F		11.075	18.408		1.00	14.61
ATOM	1554	C	ASP A		11.262	17.229	14.704	1.00	18.18
ATOM	1555	0	ASP A		12.185	16.435	14.878		13.55
ATOM	1556	CB	ASP A		10.300	18.002	16.892	1.00 1.00	4.57
ATOM	1557	CG		4 245	10.383	19.052	18.000		6.51
MOTA	1558		1 ASP A		11.487	19.485	18.364	1.00	8.18
ATOM	1559	OD:	2 ASP A	A 245	9.330	19.449	18.487	1.00	16.73
MOTA	1560	N		A 246	10.427	17.165	13.668	1.00 1.00	14.31
ATOM	1561	CA	ILE 2	A 246	10.499	16.125	12.654		
MOTA	1562	С	ILE :	A 246	11.872	16.194	12.007	1.00	17.28
MOTA	1563	0	ILE .	A 246	12.530	15.176	11.817	1.00	16.60
ATOM	1564	CB	ILE .	A 246	9.393	16.331	11.592	1.00	9.64
MOTA	1565		1 ILE		8.039	15.958	12.185	1.00	15.94
MOTA	1566	CG	2 ILE	A 246	9.643	15.492	10.337	1.00	14.00
MOTA	1567	CD	1 ILE	A 246	7.967		12.576	1.00	13.79
MOTA	1568	N	TRP	A 247	12.382		11.814	1.00	9.95
MOTA	1569	CA	TRP	A 247	13.675		11.176	1.00	8.10
MOTA	1570	C	TRP	A 247	14.777		12.008		11.11
MOTA	1571	0	TRP	A 247	15.716				6.79
ATOM	1572	CE	TRP	A 247	13.959				2.00
ATOM	1573	CG	TRP	A 247	15.372				2.00
ATOM	1574	CI	1 TRP	A 247	16.453				2.85
MOTA	1575		2 TRP		15.874				3.34
MOTA	1576	NE.	I TRP	A 247	17.596				2.00
ATOM	1577		E2 TRP	A 247	17.267				10.65
ATOM	1578		3 TRP	A 247	15.283				6.33
MOTA	1579	) C2	Z2 TRP	A 247	18.087				6.91
ATOM	1580	) C2	Z3 TRP	A 247	16.096				7.13
MOTA	1581		H2 TRP	A 247	17.480				11.35
ATOM	1582		SER	A 248	14.657				
ATOM	1583			A 248	15.636				8.73
MOTA	1584		SER	A 248	15.624				4.47
MOTA	1589			A 248	16.670		14.422		4.57
ATOM	158			A 248	15.328				8.62
ATOM				A 248	15.183				7.78
ATOM				A 249	14.433				6.41
ATOM				A 249	14.24				10.37
ATOM				A 249	14.85	2 12.455	5 12.918	3 1.00	11.86
011		_							

## FIG. 2BB

									00
MOTA	1591	0	VAL A		15.450	11.377	12.894	1.00	15.92 9.24
MOTA	1592	CB	VAL A		12.739	12.588	14.254	1.00 1.00	5.95
MOTA	1593		VAL A		12.540	11.091	13.913 15.616	1.00	6.23
MOTA	1594		VAL A		12.132	12.955 13.246	11.853	1.00	11.69
MOTA	1595	N	GLY A		14.705		10.568	1.00	2.74
MOTA	1596	CA	GLY A		15.257	12.897	10.608	1.00	7.06
MOTA	1597	C	GLY A		16.762	12.859 11.962	10.006	1.00	7.35
MOTA	1598	0	GLY A		17.374	13.821	11.297	1.00	8.01
MOTA	1599	N	CYS A		17.379	13.821	11.413	1.00	6.02
ATOM	1600	CA	CYS A		18.843 19.438	12.748	12.224	1.00	6.13
MOTA	1601	C	CYS A		20.620	12.427	12.076	1.00	6.97
MOTA	1602	0	CYS A	251 ·	19.295	15.214	12.055	1.00	11.97
ATOM	1603	CB	CYS A		19.073	16.713	11.101	1.00	16.32
MOTA	1604	SG	ILE A		18.663	12.224	13.166	1.00	6.86
MOTA	1605	N	ILE A		19.097	11.104	14.008	1.00	9.70
MOTA	1606	CA	ILE A		18.945	9.808	13.172	1.00	6.47
MOTA	1607	C	ILE A		19.870	9.012	13.062	1.00	6.74
ATOM	1608	0	ILE A		18.204	10.998	15.303	1.00	11.46
ATOM	1609	CB CG1			18.478	12.181	16.277	1.00	6.35
ATOM	1610		ILE A		18.420	9.645	15.968	1.00	9.02
ATOM	1611		ILE A		17.278	12.498	17.206	1.00	2.00
MOTA	1612	N	MET A		17.802	9.672	12.520	1.00	4.24
MOTA	1613 1614	CA	MET A		17.524	8.532	11.678	1.00	10.23
MOTA	1615	C	MET A		18.559	8.343	10.566	1.00	13.46
ATOM	1616	o	MET A		18.941	7.219	10.273	1.00	16.51
ATOM ATOM	1617	CB	MET A		16.144	8.675	11.061	1.00	10.85
MOTA	1618	CG	MET A		15.864		9.994	1.00	11.51
ATOM	1619	SD	MET A		14.242		9.425	1.00	14.35
ATOM	1620	CE	MET A		14.050	6.430	8.483	1.00	14.56
MOTA	1621	N	GLY A		18.977	9.431	9.923	1.00	14.30
ATOM	1622	CA		254 .	19.964	9.351	8.855	1.00	8.44
ATOM	1623	C	GLY A	254	21.354	9.118	9.385	1.00	9.82
ATOM	1624	0	GLY A	254	22.254	8.642	8.672	1.00	9.43
MOTA	1625	N	GLU A	255	21.582		10.625	1.00	12.87
ATOM	1626	CA	GLU A	A 255	22.873	9.291	11.247	1.00	11.63
MOTA	1627	C	GLU A	1 255	22.967		11.649	1.00	11.63
ATOM	1628	0	GLU A	A 255	24.057	7.246	11.708	1.00	12.64
ATOM	1629	CB	GLU A	A 255	23.070		12.468	1.00	11.82
MOTA	1630	CG	GLU A	A 255	24.429		13.135	1.00	. 9.96
MOTA	1631	CD	GLU A	A 255	24.688		14.267	1.00	11.66
ATOM	1632	OE		A 255	23.835		14.516	1.00	16.47
MOTA	1633	OE2	GLU A	A 255	25.749		14.906	1.00	15.14
ATOM	1634	N		A 256	21.832		11.966	1.00	12.10 14.61
ATOM	1635	CA		A 256	21.807		12.330	1.00	16.74
MOTA	1636	C		A 256	22.287		11.108	1.00	21.09
MOTA	1637	0		A 256	23.138		11.240	1.00	12.40
MOTA	1638	CB		A 256	20.387		12.784		12.40
MOTA	1639	CG		A 256	20.029			1.00 1.00	23.36
MOTA	1640	SD		A 256	18.257				16.21
MOTA	1641	CE		A 256	18.048				17.44
ATOM	1642	N		A 257	21.816				18.71
MOTA	1643	CA		A 257	22.184				20.14
MOTA	1644			A 257	23.534				23.29
MOTA	1645			A 257	24.335				19.20
MOTA	1646			A 257	21.108				14.26
MOTA	1647		1 VAL		19.684				21.30
MOTA	1648		2 VAL		21.304				19.80
ATOM	1649	N	ARG	A 258	23.80	0.343	0.102	1.00	

## FIG. 2CC

MOTA	1650	CA .	ARG A	258		5.057	6.854	7.559	1.00	19.39
MOTA	1651	C .	ARG A	258		6.292	6.724	8.448	1.00	22.54
MOTA	1652	0	ARG A	258		7.426	6.741	7.952	1.00	25.87
MOTA	1653	CB	ARG A	258	2	4.880	8.314	7.149	1.00	19.45
MOTA	1654	CG	ARG A	258	2	6.141	8.897	6.558	1.00	21.22
MOTA	1655	CD	ARG A	258	2	6.013	10.368	6.322	1.00	24.45
MOTA	1656		ARG A			5.130	10.640	5.202	1.00	28.85
ATOM	1657	CZ	ARG A	258		5.013	11.829	4.629	1.00	30.35
MOTA	1658		ARG A			25.737	12.844	5.097	1.00	33.58
MOTA	1659		ARG A			4.192	12.005	3.591	1.00	26.26
MOTA	1660		HIS A			26.068	6.557	9.750	1.00	25.71 27.73
MOTA	1661		HIS A			27.118	6.449	10.785	1.00	28.00
MOTA	1662		HIS A			8.103	7.621	10.883	1.00	29.52
MOTA	1663	0	HIS A			29.309	7.469	11.103	1.00	26.36
ATOM	1664	CB	HIS A			27.805	5.055	10.818	1.00	20.38
MOTA	1665	CG	HIS A			26.879	3.943	11.229	1.00	22.41
MOTA	1666		HIS A			26.446	3.763	12.527	1.00	20.61
MOTA	1667		HIS A			26.213	3.021	10.492	1.00	19.01
MOTA	1668		HIS A			25.549	2.795	12.566	1.00	16.47
MOTA	1669	NE2	HIS A			25.387	2.329	11.347	1.00	29.63
MOTA	1670	N	LYS A			27.539	8.801	10.696	1.00	30.40
MOTA	1671	CA	LYS A			28.243	10.066	10.819	1.00 1.00	26.07
MOTA	1672	C	LYS A			27.206	11.193	10.863	1.00	24.49
ATOM	1673	0	LYS A			26.077	11.041	10.380 9.721	1.00	33.87
MOTA	1674	CB	LYS F			29.291	10.267	10.297	1.00	40.62
MOTA	1675	CG	LYS F			30.720	10.237	11.428	1.00	46.13
MOTA	1676	CD.	LYS F			30.871	11.271	12.733	1.00	48.31
MOTA	1677	CE	LYS A			31.363	10.641	13.894	1.00	47.46
MOTA	1678	NZ	LYS A			30.799	11.393	11.542	1.00	22.60
MOTA	1679	N	ILE A			27.532	12.283	11.642	1.00	19.96
MOTA	1680	CA		A 261		26.578	14.027	10.272	1.00	17.51
MOTA	1681	C		A 261		26.353	14.420	9.585	1.00	17.46
ATOM	1682	0		A 261		27.286	14.436	12.719	1.00	18.47
MOTA	1683	CB		A 261		27.007 27.110	13.771	14.090	1.00	15.26
MOTA	1684	CG1		A 261		25.959	15.561	12.833	1.00	20.19
MOTA	1685	CG2		A 261		28.022	14.488	15.024	1.00	19.17
MOTA	1686	CD1		A 261		25.022	14.045	9.871	1.00	17.50
ATOM	1687	N		A 262 A 262		24.659	14.617	8.607	1.00	18.94
ATOM	1688	CA		A 262		25.138	16.066	8.372	1.00	20.67
ATOM	1689	C		A 262		25.938	16.328	7.466	1.00	22.13
ATOM	1690	0		A 262		23.128	14.559	8.550	1.00	13.08
ATOM	1691	CB		A 262		22.423	13.385	7.868	1.00	14.46
ATOM	1692	CG	LEU .			22.952	12.062	8.369	1.00	14.89
MOTA	1693		LEU .			20.942	13.488	8.066	1.00	7.56
MOTA	1694		DUE.	A 263		24.702	16.986	9.226		20.64
ATOM	1695	N		A 263		25.034		9.069		20.07
MOTA	1696	CA	PHE .	A 263		25.969		10.151		20.50
MOTA	1697	C		A 263		25.579		10.959		20.92
ATOM	1698			A 263		23.719		8.998		18.23
ATOM	1699			A 263		22.697		8.022		14.68
ATOM	1700		PHE	A 263		22.953		6.653		12.98
MOTA	1701	רנט. רנו	PHE	A 263		21.484		8.473		9.26
ATOM	1702	CD2	PHE	A 263		22.016		5.760		8.44
ATOM	1703	CEI	PHE	A 263		20.551		7.584		5.41
ATOM	1704		DUE!	A 263		20.824		6.222		3.79
MOTA	1705 1706			A 264		27.229		10.159		19.70
ATOM				A 264		28.184		11.160		23.64
ATOM	1707			A 264		28.643				25.18
ATOM	1708	_	FRO							



## FIG. 2DD

										05 05
ATOM	1709	0	PRO	A	264	28.040	21.173	10.185	1.00	25.01
MOTA	1710	CB	PRO	Α	264	29.339	18.026	11.024	1.00	22.88
MOTA	1711	CG	PRO			29.272	17.638	9.570	1.00	20.00
						27.814	17.464	9.341	1.00	19.45
MOTA	1712	CD	PRO							27.92
ATOM	1713	N	GLY			29.741	20.807	11.606	1.00	
MOTA	1714	CA	GLY	Α	265	30.254	22.160	11.447	1.00	32.00
MOTA	1715	C	GLY	A	265	31.038	22.802	12.586	1.00	32.60
MOTA	1716	0	GLY	Α	265	32.079	22.306	13.047	1.00	33.24
ATOM	1717	N	ARG			30.571	23.976	12.985	1.00	31.55
			ARG			31.197	24.726	14.058	1.00	32.94
ATOM	1718	CA								
MOTA	1719	С	ARG			30.200	25.778	14.485	1.00	33.00
MOTA	1720	0	ARG	Α	266	30.019	26.043	15.670	1.00	31.47
MOTA	1721	CB	ARG	Α	266	32.486	25.401	13.576	1.00	34.09
MOTA	1722	CG	ARG	Α	266	32.327	26.393	12.414	1.00	33.36
ATOM	1723	CD	ARG	A	266	33.694	26.964	12.003	1.00	31.74
	1724	NE	ARG			33.653	27.527	10.659	1.00	30.39
ATOM								9.900	1.00	24.25
MOTA	1725	CZ	ARG			34.718	27.748			
MOTA	1726		ARG			35.935	27.483	10.346	1.00	25.66
ATOM	1727	NH2	ARG	A	266	34.552	28.132	8.648	1.00	25.54
MOTA	1728	N	ASP	A	267	29.513	26.327	13.491	1.00	33.80
MOTA	1729	CA	ASP	Α	267	28.532	27.358	13.714	1.00	30.50
MOTA	1730	C	ASP			27.459		12.656	1.00	26.92
						27.676	26.614	11.627	1.00	26.99
MOTA	1731	0	ASP							37.49
ATOM	1732	CB	ASP			29.198	28.723	13.611	1.00	
MOTA	1733	CG	ASP	Α	267	28.284	29.820	14.030	1.00	40.83
MOTA	1734	OD1	ASP	A	267	27.949	30.663	13.175	1.00	44.75
MOTA	1735	OD2	ASP	Α	267	27.844	29.799	15.202	1.00	44.89
ATOM	1736	N	TYR			26.330	27.875	12.907	1.00	25.13
ATOM	1737	CA.	TYR			25.173	27.877	12.030	1.00	24.71
								10.557	1.00	25.16
MOTA	1738	C			268	25.444	28.208			
MOTA	1739	0	TYR			24.569	28.030	9.715	1.00	26.18
ATOM	1740	CB	TYR	Α	268	24.173	28.889	12.551	1.00	23.88
ATOM	1741	CG	TYR	Α	268	23.318	28.454	13.701	1.00	25.55
ATOM	1742	CD1	TYR	Α	268	23.505	27.243	14.348	1.00	24.78
MOTA	1743		TYR			22.257	29.242	14.100	1.00	28.07
MOTA	1744		TYR			22.629	26.834	15.367	1.00	26.43
		CE2				21.395	28.852	15.101	1.00	29.67
ATOM	1745									28.32
MOTA	1746	$\mathbf{cz}$			268	21.576	27.652	15.734	1.00	
ATOM	1747	OH	TYR	A	268	20.679	27.306	16.720	1.00	30.67
MOTA	1748	N	ILE	Α	269	26.610	28.772	10.261	1.00	25.39
ATOM	1749	CA	ILE	A	269	26.971	29.136	8.891	1.00	24.88
ATOM	1750	C	ILE	Α	269	27.425	27.850	8.230	1.00	24.23
MOTA	1751	ō			269	26.853	27.412	7.235	1.00	23.59
						28.196	30.118	8.842	1.00	24.89
MOTA	1752	CB		_	269					
MOTA	1753		ILE			27.904	31.463	9.519	1.00	24.46
ATOM	1754	CG2	ILE	A	269	28.638	30.324	7.411	1.00	25.64
ATOM	1755	CD1	ILE	Α	269	26.977	32.369	8.767	1.00	21.32
MOTA	1756	N	ASP	Α	270	28.468	27.268	8.823	1.00	24.17
ATOM	1757	CA	ASP			29.099	26.020	8.374	1.00	26.59
ATOM	1758	C			270	28.009	24.978	8.119	1.00	26.04
					270	27.804	24.492	7.003	1.00	26.38
ATOM	1759	0								
MOTA	1760	CB			270	30.058	25.526	9.483	1.00	25.96
MOTA	1761	CG	ASP	Α	270	31.198	24.667	8.959	1.00	23.06
MOTA	1762	OD1	ASP	Α	270	32.246	24.588	9.624	1.00	19.74
ATOM	1763	OD2	ASP	A	270	31.055	24.060	7.880	1.00	31.30
ATOM	1764	N			271	27.234	24.764	9.168	1.00	25.91
ATOM	1765	CA			271	26.133	23.820	9.211	1.00	24.57
MOTA	1766	C			271	25.089	24.056	8.121	1.00	23.81
						24.563	23.103		1.00	25.98
ATOM	1767	0	CILIN	A	271	24.503	23.103	7.549	T.00	23.90



#### FIG. 2EE

MOTA	1768	CB	GLN A	A 271	25	5.501	23.926	10.593	1.00	25.83
ATOM	1769	CG	GLN A	A 271	24	1.574	22.818	10.984	1.00	27.68
MOTA	1770	CD	GLN A	A 271	24	1.013	23.050	12.357	1.00	26.89
ATOM	1771	OE1	GLN Z	A 271	24	1.725	23.485	13.281	1.00	23.91
ATOM	1772			A 271	2:	2.726	22.781	12,504	1.00	25.73
MOTA	1773	N		A 272		1.763	25.311	7.830	1.00	22.13
				A 272		3.783	25.576	6.788	1.00	19.21
MOTA	1774						25.204	5.457	1.00	18.17
ATOM	1775	C		A 272		4.419				16.56
ATOM	1776	0		A 272		3.751	24.749	4.534	1.00	
MOTA	1777	CB		A 272		3.358	27.037	6.775	1.00	17.37
MOTA	1778	CG	TRP 2	A 272	2:	2.364	27.377	5.686	1.00	13.75
MOTA	1779	CD1	TRP 3	A 272	2	2.557	28.269	4.659	1.00	15.40
ATOM	1780	CD2	TRP .	A 272	2	1.006	26.884	5.535	1.00	15.21
ATOM	1781	NE1	TRP .	A 272	2	1.412	28.374	3.897	1.00	16.90
MOTA	1782	CE2	TRP	A 272	2	0.446	27.542	4.408	1.00	14.39
ATOM	1783	CE3		A 272		0.217	25.965	6.241	1.00	14.65
MOTA	1784	CZ2		A 272		9.130	27.298	3.971	1.00	14.28
						8.909	25.725	5.808	1.00	13.40
ATOM	1785	CZ3		A 272			26.391	4.686	1.00	16.96
MOTA	1786	CH2		A 272		8.377		5.377	1.00	19.02
MOTA	1787	N		A 273		5.729	25.353			
MOTA	1788	CA		A 273		6.408	25.013	4.146	1.00	22.48
MOTA	1789	C	ASN .	A 273	2	6.158	23.544	3.866	1.00	22.47
ATOM	1790	0	ASN	A 273	2	5.748	23.187	2.759	1.00	22.01
MOTA	1791	CB	ASN	A 273	2	7.912	25.316	4.238	1.00	22.52
ATOM	1792	CG	ASN	A 273	2	8.227	26.798	4.062	1.00	21.44
ATOM	1793	OD1	ASN	A 273	2	7.348	27.621	3.781	1.00	21.70
ATOM	1794	ND2		A 273	2	9.488	27.143	4.209	1.00	24.93
ATOM	1795	N		A 274		6.278	22.719	4.914	1.00	23.46
	1796	CA		A 274		6.072	21.271	4.805	1.00	18.10
ATOM						4.626	20.942	4.475	1.00	18.00
ATOM	1797	C		A 274			19.937	3.833	1.00	22.35
MOTA	1798	0_		A 274		4.361		6.093	1.00	15.27
ATOM	1799	CB		A 274		6.451	20.566		1.00	14.30
MOTA	1800	CG		A 274		7.811	20.904	6.600		
MOTA	1801	CD		A 274		8.900	20.434	5.691	1.00	19.69
MOTA	1802	CE	LYS	A 274	3	0.186	20.267	6.502	1.00	24.70
ATOM	1803	NZ	t LYS	A 274	3	1.204	19.327	5.896	1.00	31.99
MOTA	1804	N	VAL	A 275	2	3.680	21.770	4.898	1.00	18.18
ATOM	1805	CA	$\nabla AL$	A 275	2	2.286	21.487	4.581	1.00	20.59
MOTA	1806	С	VAL	A 275	2	1.968	21.762	3.110	1.00	23.32
ATOM	1807	0	VAL	A 275	2	1.204	21.023	2.486	1.00	25.67
ATOM	1808	CB		A 275	2	1.282	22.310	5.449	1.00	17.97
MOTA	1809			A 275		9.836	21.995	5.045	1.00	15.19
				A 275		1.498	22.025	6.928	1.00	19.77
MOTA	1810					2.580	22.801	2.547	1.00	23.82
MOTA	1811	N		A 276				1.164	1.00	20.92
MOTA	1812	CA		A 276		2.320	23.168	0.147	1.00	20.60
ATOM	1813	С		A 276		3.120	22.356		1.00	23.64
MOTA	1814	0		A 276		22.640	22.087	-0.952		
MOTA	1815	CB		A 276		22.506	24.703	0.926	1.00	18.18
MOTA	1816	CG1	ILE	A 276		23.916	25.139	1.336	1.00	18.15
ATOM	1817	CG2	ILE	A 276	2	21.429	25.464	1.643	1.00	9.12
MOTA	1818	CD1	ILE	A 276		24.426	26.400	0.674	1.00	16.28
MOTA	1819	N		A 277	2	24.313	21.923	0.511	1.00	20.50
ATOM	1820	CA		A 277		25.091		-0.423	1.00	23.41
ATOM	1821	C		A 277		24.653	19.705	-0.550	1.00	28.35
ATOM	1822	o		A 277		25.080	19.002		1.00	34.25
		CB		A 277		26.572	21.265			19.67
MOTA	1823					27.058		0.982		24.35
MOTA	1824	CG		A 277						30.31
MOTA	1825	CD		A 277		28.553				35.18
ATOM	1826	OEI	. GLU	A 277	-	29.232	T3.2T0	1.313	1.00	0ء. د د

## FIG. 2FF

	1007	OEO	OT II A 277	29.050	21.704	1.058	1.00	28.91
ATOM	1827		GLU A 277 GLN A 278	23.795	19.245	0.350	1.00	26.32
MOTA	1828	N	GLN A 278	23.316	17.880	0.283	1.00	22.89
ATOM	1829	CA C	GLN A 278	21.888	17.806	-0.235	1.00	22.44
MOTA	1830	0	GLN A 278	21.580	16.978	-1.089	1.00	23.76
MOTA	1831	СВ	GLN A 278	23.422	17.212	1.649	1.00	23.63
MOTA	1832	CG	GLN A 278	24.850	17.022	2.111	1.00	25.91
ATOM	1833 1834	CD	GLN A 278	24.918	16.301	3.446	1.00	29.41
ATOM	1835	OE1		24.521	15.139	3.552	1.00	26.75
ATOM ATOM	1836	NE2	GLN A 278	25.407	16.993	4.476	1.00	30.71
ATOM	1837	N	LEU A 279	21.018	18.676	0.263	1.00	20.12
MOTA	1838	CA	LEU A 279	19.628	18.681	-0.171	1.00	20.56
ATOM	1839	C	LEU A 279	19.369	19.804	-1.200	1.00	20.66
ATOM	1840	ō	LEU A 279	18.273	19.908	-1.758	1.00	20.40
ATOM	1841	CB	LEU A 279	18.678	18.852	1.036	1.00	19.86
MOTA	1842	CG	LEU A 279	18.904	18.176	2.405	1.00	19.25
ATOM	1843		LEU A 279	17.786	18.595	3.383	1.00	12.82
ATOM	1844		LEU A 279	18.967	16.661	2.278	1.00	17.53
ATOM	1845	N	GLY A 280	20.365	20.663	-1.402	1.00	21.53
ATOM	1846	CA	GLY A 280	20.243	21.768	-2.338	1.00	21.98
ATOM	1847	C	GLY A 280	19.735	23.072	-1.749	1.00	24.54
ATOM	1848	Ō	GLY A 280	19.401	23.165	-0.569	1.00	26.75
ATOM	1849	N	THR A 281	19.648	24.095	-2.585	1.00	24.49
MOTA	1850	CA	THR A 281	19.174	25.394	-2.145	1.00	28.73
MOTA	1851	C	THR A 281	17.633	25.347	-2.013	1.00	30.15
ATOM	1852	0	THR A 281	16.956	24.708	-2.818	1.00	31.24
MOTA	1853	CB	THR A 281	19.675	26.539	-3.129	1.00	30.04
MOTA	1854	OG1	THR A 281	21.040	26.284	-3.514	1.00	29.30
ATOM	1855	CG2	THR A 281	19.649	27.912	-2.450	1.00	31.80
MOTA	1856	N	PRO A 282	17.074	25.969	-0.951	1.00	30.63
MOTA	1857	CA	PRO A 282	15.621	25.973	-0.742	1.00	31.39
MOTA	1858	C	PRO A 282	14.790	26.593	-1.860	1.00	35.04 34.15
ATOM	1859	0	PRO A 282	15.137	27.622	-2.442	1.00	27.71
MOTA	1860	CB	PRO A 282	15.465	26.736	0.576	1.00	28.19
MOTA	1861	CG	PRO A 282	16.711	26.411	1.309	1.00	26.87
MOTA	1862	$^{\rm CD}$	PRO A 282	17.763	26.542	0.215	1.00	39.56
MOTA	1863	N	CYS A 283	13.651	25.954	-2.102	1.00 1.00	42.11
MOTA	1864	CA	CYS A 283	12.678	26.348	-3.116	1.00	41.47
MOTA	1865	C	CYS A 283	12.300	27.819	-3.079	1.00	39.65
MOTA	1866	0	CYS A 283	12.033	28.363	-2.022 -2.936	1.00	45.67
MOTA	1867	CB	CYS A 283	11.401	25.508 25.546	-1.228	1.00	49.59
MOTA	1868	SG	CYS A 283	10.669 12.415	28.507	-4.220	1.00	43.20
MOTA	1869	N	PRO A 284	12.415	29.933	-4.341	1.00	43.55
MOTA	1870	CA	PRO A 284	10.618	30.191	-3.925	1.00	43.04
MOTA	1871	C	PRO A 284	9.676	30.140	-4.735	1.00	43.04
MOTA	1872	0	PRO A 284 PRO A 284	12.321	30.241	-5.826	1.00	44.13
MOTA	1873	CB	PRO A 284		28.883	-6.460	1.00	47.78
MOTA	1874	CG	PRO A 284	13.306	28.106	-5.318	1.00	44.72
MOTA	1875	CD	ALA A 285		30.388	-2.619	1.00	40.82
MOTA	1876	N CA	ALA A 285		30.634	-1.951	1.00	39.42
MOTA	1877 1878	CA	ALA A 285		30.601	-0.465	1.00	39.31
ATOM ATOM	1879	0	ALA A 285			0.307	1.00	41.09
ATOM	1880	CB	ALA A 285			-2.275		39.41
ATOM	1881	N	PHE A 286			-0.096		36.13
MOTA	1882	CA				1.261	1.00	29.31
ATOM	1883	C	PHE A 286		_	1.819		29.93
MOTA	1884	ō	PHE A 286			2.923	1.00	27.02
ATOM	1885				28.251	1.237	1.00	25.30
				•				

## FIG. 2GG

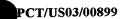
					30 446	27 021	2.581	1.00	18.21
MOTA	1886		PHE A 2		12.446 11.621	27.931 27.534	3.624	1.00	18.09
MOTA	1887		PHE A 2		13.811	28.035	2.805	1.00	15.83
MOTA	1888		PHE A 2		12.154	27.245	4.887	1.00	18.38
MOTA	1889		PHE A 2		14.357	27.754	4.052	1.00	18.25
MOTA	1890		PHE A 2		13.533	27.357	5.097	1.00	15.03
MOTA	1891		PHE A 2		12.340	31.256	1.019	1.00	32.98
MOTA	1892		MET A		13.021	32.485	1.411	1.00	35.50
MOTA	1893		MET A		12.110	33.659	1.797	1.00	35.57
MOTA	1894		MET A		12.566	34.586	2.456	1.00	36.21
MOTA	1895		MET A :		13.986	32.935	0.312	1.00	37.48
MOTA	1896		MET A		15.377	32.320	0.388	1.00	38.29
MOTA	1897		MET A		15.506	30.652	-0.248	1.00	42.69
ATOM	1898		MET A		15.218	30.918	-1.938	1.00	39.17
ATOM	1899		LYS A		10.833	33.607	1.428	1.00	36.32
MOTA	1900		LYS A		9.895	34.678	1.753	1.00	37.98
ATOM	1901		LYS A		9.604	34.812	3.251	1.00	41.25
MOTA	1902		LYS A		9.347	35.919	3.748	1.00	42.92
MOTA	1903		LYS A		8.573	34.480	1.004	1.00	39.11
MOTA	1904	CB	LYS A		8.479	35.161	-0.371	1.00	42.11
ATOM	1905	CD CD	LYS A		9.372	34.565	-1.463	1.00	44.65
ATOM	1906	CE	LYS A		9.066	35.248	-2.815	1.00	47.02
ATOM	1907	NZ	LYS A		9.881	34.775	-3.985	1.00	45.67
ATOM	1908	NZ N	LYS A		9.611	33.691	3.969	1.00	41.56
MOTA	1909	CA	LYS A		9.345	33.722	5.407	1.00	40.78
MOTA	1910 1911	C	LYS A		10.626	33.990	6.206	1.00	39.17
MOTA	1911	0	LYS A		10.643	33.955	7.452	1.00	38.50
ATOM	1912	СВ	LYS A		8.692	32.415	5.850	1.00	43.27
MOTA	1914	CG	LYS A		7.262	32.219	5.330	1.00	47.51
ATOM ATOM	1915	CD	LYS A		6.305	33.345	5.782	1.00	51.55
ATOM	1916	CE	LYS A		6.180	33.475	7.313	1.00	52.02
ATOM	1917	NZ	LYS A		7.275	34.267	7.960	1.00	54.69
ATOM	1918	N	LEU A		11.670	34.336	5.462	1.00	36.37
ATOM	1919	CA	LEU A		12.992	34.622	6.001	1.00	36.82
ATOM	1920	C	LEU A		13.167	36.136	6.198	1.00	37.74
MOTA	1921	ō	LEU A		13.092	36.896	5.227	1.00	39.91
MOTA	1922	СВ	LEU A		14.013	34.103	4.993	1.00	32.06
MOTA	1923	CG	LEU A	290	15.236	33.276	5.380	1.00	32.32
MOTA	1924	CD1	LEU A	290	15.046	32.512	6.675	1.00	28.02
ATOM	1925	CD2			15.564		4.224	1.00	27.96
MOTA	1926	N	GLN A	291	13.399		7.438	1.00	39.04
MOTA	1927	CA	GLN A	291	13.584	38.021	7.711	1.00	38.20
MOTA	1928	C	GLN A	291	14.561		6.664	1.00	37.52
ATOM	1929	0	GLN A	291	15.495		6.267	1.00	36.29
MOTA	1930	CB	GLN A		14.142		9.123	1.00	39.70
ATOM	1931	CG	GLN A	291	14.008		9.641		43.34
ATOM	1932	CD	GLN A		12.729		10.459		43.23
MOTA	1933	OE1	GLN A		12.426		11.375		45.26
MOTA	1934	NE2			11.989		10.137		40.70 35.64
MOTA	1935	N	PRO A		14.339		6.193		34.65
ATOM	1936	CA	PRO A		15.129		5.179		35.33
MOTA	1937	C	PRO A		16.634		5.292		33,35
ATOM	1938	0	PRO A		17.325		4.287		35.18
MOTA	1939	CB	PRO A		14.665		5.353		34.12
MOTA	1940		PRO A		13.22				35.37
ATOM	1941	CD	PRO A		13.282				37.57
MOTA	1942		THR A		17.146				39.75
MOTA	1943		THR A		18.58	5 40.230			39.73
MOTA	1944	C	THR A	. 293	19.05	0 <sub>.</sub> 38.772	6.627	1.00	37.20

# FIG. 2HH

MOTA	1945	0	THR	A	293	20.210	38.506	6.289	1.00	37.75
ATOM	1946	CB	THR			19.043	40.827	8.035	1.00	42.63
ATOM	1947	OG1				18.061	41.766	8.512	1.00	47.19
ATOM	1948	CG2	THR	A	293	20.419	41.515	7.852	1.00	40.06
MOTA	1949	N	VAL	A	294	18.159	37.843	6.988	1.00	36.77
MOTA	1950	CA	VAL	A	294	18.464	36.413	6.956	1.00	34.85
ATOM	1951	С	VAL	Α	294	18.343	35.930	5.536	1.00	33.86
MOTA	1952	0	VAL	А	294	19.169	35.154	5.060	1.00	33.38
ATOM	1953	CB	VAL	Α	294	17.450	35.566	7.738	1.00	34.91
MOTA	1954	CG1	VAL	A	294	17.953	34.144	7.816	1.00	35.42
MOTA	1955	CG2	VAL	A	294	17.213	36.124	9.127	1.00	37.51
MOTA	1956	N	ARG	Α	295	17.297	36.404	4.867	1.00	33.96
ATOM	1957	CA	ARG	A	295	17.020	36.035	3.492	1.00	34.52
MOTA	1958	С	ARG	Α	295	18.099	36.552	2.544	1.00	36.07
MOTA	1959	0	ARG	Α	295	18.361	35.940	1.502	1.00	37.40
MOTA	1960	CB	ARG	A	295	15.636	36.534	3.070	1.00	34.81
MOTA	1961	CG	ARG	A	295	15.619	37.953	2.559	1.00	36.10
MOTA	1962	CD	ARG	A	295	14.402	38.189	1.706	1.00	30.72
MOTA	1963	NE	ARG	A	295	13.204	38.284	2.511	1.00	26.85
MOTA	1964	$\mathbf{cz}$	ARG	Α	295	11.981	38.371	2.008	1.00	30.88
MOTA	1965	NH1	ARG	A	295 ·	11.790	38.366	0.694	1.00	33.56
ATOM	1966	NH2	ARG	A	295	10.946	38.518	2.822	1.00	34.68
MOTA	1967	N	ASN	Α	296	18.736	37.666	2.899	1.00	35.96
MOTA	1968	CA	ASN	Α	296	19.790	38.224	2.072	1.00	33.95
MOTA	1969	С	ASN	Α	296	20.923	37.225	1.996	1.00	33.60
MOTA	1970	0	ASN	A	296	21.366	36.868	0.899	1.00	34.00
ATOM	1971	СВ	ASN	Α	296	20.333	39.510	2.680	1.00	36.06
ATOM	1972	CG	ASN	Α	296	21.513	40.050	1.906	1.00	35.72
MOTA	1973	OD1	ASN	A	296	21.331	40.659	0.858	1.00	36.39
MOTA	1974	ND2	ASN	A	296	22.732	39.772	2.381	1.00	34.76
ATOM	1975	N	TYR	A	297	21.408	36.802	3.172	1.00	31.97
ATOM	1976	CA	TYR	Α	297	22.498	35.819	3.309	1.00	29.60
MOTA	1977	С	TYR	A	297	22.218	34.521	2.549	1.00	28.11
MOTA	1978	0	TYR	Α	297	23.084	34.020	1.840	1.00	28.70
MOTA	1979	CB	TYR	A	297	22.740	35.481	4.795	1.00	26.28
ATOM	1980	CG	TYR	Α	297	23.722	34.341	5.021	1.00	26.96
MOTA	1981	CD1	TYR	Α	297	25.091	34.533	4.887	1.00	25.56
MOTA	1982	CD2	TYR	Α	297	23.277	33.061	5.346	1.00	27.53
MOTA	1983	CE1	TYR	Α	297	25.986	33.486	5.061	1.00	25.70
ATOM	1984	CE2	TYR	A	297	24.169	32.012	5.518	1.00	26.17
ATOM	1985	CZ	TYR	Α	297	25.520	32.229	5.367	1.00	25.43
MOTA	1986	OH	TYR	A	297	26.406	31.179	5.452	1.00	28.49
MOTA	1987	N	VAL	Α	298	21.006	33.996	2.711	1.00	28.24
MOTA	1988	CA	VAL	A	298	20.569	32.750	2.102	1.00	27.73
MOTA	1989	C	VAL	Α	298	20.413	32.855	0.589	1.00	29.27
MOTA	1990	0	VAL	A	298	20.990	32.055	-0.158	1.00	28.77
MOTA	1991	CB	VAL	A	298	19.238	32.288	2.758	1.00	26.32
MOTA	1992	CG1	LAV	Α	298	18.614	31.158	1.992	1.00	29.24
MOTA	1993	CG2	VAL	A	298	19.490	31.872	4.209	1.00	29.06
MOTA	1994	N	GLU	Α	299	19.687	33.876	0.131	1.00	30.27
MOTA	1995	CA			299	19.452	34.088	-1.295	1.00	28.19
MOTA	1996	C			299	20.767	34.320	-1.981	1.00	27.95
MOTA	1997	0			299	20.897	34.065	-3.171	1.00	29.01
ATOM	1998	CB			299	18.562	35.302	-1.539	1.00	28.56
ATOM	1999	CG			.299	17.151	35.179	-0.992	1.00	32.18
MOTA	2000	CD	·GLU			16.093		-1.971	1.00	36.34
ATOM	2001		GLU			14.993		-1.516	1.00	37.16
MOTA	2002		GLU			16.356		-3.199	1.00	37.87
ATOM	2003	N			300	21.746		-1.218	1.00	29.48

## FIG. 2II

			3 C) 7	200	าว	.067	35.083	-1.747	1.00	27.96
MOTA	2004	CA	ASN A				34.004	-1.491	1.00	26.74
MOTA	2005	C	ASN A			.104	34.304	-1.451	1.00	27.37
MOTA	2006	0	ASN A			5.291		-1.191	1.00	32.01
MOTA	2007	CB	ASN A			.581	36.412	-1.649	1.00	34.99
MOTA	2008	CG	ASN A			.759	37.609			40.39
ATOM	2009	OD1	ASN A			3.608	38.572	-0.908	1.00	
MOTA	2010	ND2	ASN A	300		2.236	37.560	-2.874	1.00	40.11
ATOM	2011	N	ARG A	301	23	3.675	32.754	-1.323	1.00	29.11
MOTA	2012	CA	ARG A	301	24	1.618	31.646	-1.070	1.00	29.04
ATOM	2013	С	ARG A	301	24	1.922	30.886	-2.369	1.00	28.33
MOTA	2014	0	ARG A	301	24	1.077	30.856	-3.272	1.00	25.54
ATOM	2015	CB	ARG A	301	24	1.026	30.593	-0.083	1.00	25.95
ATOM	2016	CG	ARG A	301	23	3.797	31.018	1.342	1.00	21.29
ATOM	2017	CD	ARG A	301	2	5.069	31.501	1.958	1.00	20.39
ATOM	2018	NE	ARG A	301	20	5.164	30.562	1.784	1.00	20.66
MOTA	2019	CZ	ARG A		2	7.443	30.867	1.989	1.00	26.05
ATOM	2020		ARG A		2'	7.775	32.094	2.365	1.00	29.37
	2021	NH2				8.397	29.946	1.873	1.00	27.83
ATOM	2022	N	PRO A			6.152	30.314	-2.489	1.00	29.03
ATOM		CA	PRO A			6.561	29.535	-3.668	1.00	31.83
MOTA	2023		PRO A			5.470	28.465	-3.932	1.00	34.72
ATOM	2024	C	PRO A			5.181	27.637	-3.054	1.00	36.10
ATOM	2025	0				7.894	28.877	-3.225	1.00	29.18
MOTA	2026	CB	PRO A			8.211	29.449	-1.841	1.00	27.99
MOTA	2027	CG	PRO A			7.323	30.659	-1.666	1.00	27.00
MOTA	2028	CD	PRO A			4.825	28.519	-5.100	1.00	35.33
MOTA	2029	N	ALA A				27.574	-5.425	1.00	32.36
MOTA	2030	CA	ALA A			3.756		-5.551	1.00	32.18
MOTA	2031	С	ALA A			4.194	26.103	-5.874	1.00	28.91
MOTA	2032	Ο.	ALA A			5.361	25.784		1.00	31.16
MOTA	2033	CB	ALA A			2.960	28.038	-6.637		33.00
ATOM	2034	N	TYR A			3.245	25.230	-5.188	1.00	29.61
MOTA	2035	CA	TYR A			3.394	23.765	-5.163	1.00	29.37
ATOM	2036	С	TYR A	304		2.126	23.055	-5.655	1.00	
MOTA	2037	0	TYR A			1.004	23.459	-5.333	1.00	27.81
ATOM	2038	CB	TYR A	304	2	3.666	23.284	-3.731	1.00	24.77
MOTA	2039	CG	TYR A	304	2	5.116	23.200	-3:363	1.00	24.50
MOTA	2040	CD1	L TYR A	304	2	5.752	24.240	-2.702	1.00	25.72
MOTA	2041	CD2	TYR A	304	. 2	5.857	22.065	-3.661	1.00	26.30
MOTA	2042	CE1	L TYR A	304	2	7.095	24.153	-2.345	1.00	29.74
ATOM	2043	CE2	TYR A	304	2	7.194	21.962	-3.317	1.00	28.89
ATOM	2044	cz	TYR A	304	2	7.817	23.012	-2.659	1.00	32.70
ATOM	2045	ОН	TYR A	304	2	9.171	22.939	-2.356	1.00	33.67
ATOM	2046	N		¥ 305	2	22.305	22.025	-6.478	1.00	29.27
ATOM	2047	CA	ALA A	305	2	1.167	21.253	-6.968	1.00	28.38
ATOM	2048	C		305	2	20.752	20.290	-5.867	1.00	26.04
ATOM	2049	ō		A 305		L9.581	19.934	-5.738	1.00	23.89
ATOM	2050	СВ		A 305		21.562		-8.210	1.00	29.32
ATOM	2051	N		A 306		21.755		-5.106	1.00	24.87
	2052	CA		A 306		21.553		-4.005	1.00	27.80
ATOM	2052	C		A 306		21.401		-4.503		27.75
ATOM				A 306		20.829		-5.572		30.73
MOTA	2054	O		A 307		21.908				25.91
ATOM	2055	N		A 307		21.812				22.59
MOTA	2056	CA				20.478				23.95
MOTA	2057	C	TIEO 1	A 307		20.476 19.732				24.98
ATOM	2058	0		A 307		19./3 <i>2</i> 22.854				18.77
MOTA	2059	CB		A 307		22.854 24.229				20.81
ATOM	2060	CG		A 307					_	22.83
MOTA	2061		1 LEU			25.034				23.95
ATOM	2062	CD	2 LEU	A 307		24.864	15.284	-4.5/1		22.55



# FIG. 2JJ

MOTA	2063	N	THR A		0.179	13.429	-4.529	1.00	24.56
MOTA	2064	CA	THR A		8.945	12.702	-4.269	1.00	22.19 17.31
MOTA	2065	C	THR A	308	9.191	11.838	-3.028	1.00 1.00	13.75
ATOM	2066	0	THR A		0.331	11.552	-2.657	1.00	24.54
MOTA	2067	CB	THR A		8.511	11.774	-5.461	1.00	24.50
MOTA	2068	OG1	THR A		9.560	10.851	-5.778 -6.681	1.00	21.46
MOTA	2069	CG2	THR A		8.121	12.590	-2.425	1.00	17.90
MOTA	2070	N	PHE A		8.111	11.383	-1.248	1.00	23.22
MOTA	2071	CA	PHE A		8.235	10.560 9.257	-1.457	1.00	25.08
MOTA	2072	C	PHE A		.8.974 .9.653	8.804	-0.542	1.00	25.85
MOTA	2073	0	PHE A		.6.887	10:374	-0.578	1.00	21.29
MOTA	2074	CB	PHE A		6.452	11.591	0.164	1.00	22.18
ATOM	2075	CG	PHE A		15.864	12.659	-0.510	1.00	21.34
MOTA	2076	CD1			16.736	11.723	1.517	1.00	21.79
ATOM	2077	CD2	PHE A		15.572	13.856	0.158	1.00	22.53
ATOM	2078				L6.452	12.909	2.195	1.00	22.27
ATOM	2079	CE2 CZ	PHE A		L5.866	13.979	1.514	1.00	22.02
ATOM	2080	N	PRO A		18.841	8.625	-2.640	1.00	25.50
ATOM	2081	CA	PRO A		19.543	7.364	-2.888	1.00	22.46
MOTA	2082	C	PRO A		21.041	7.566	-2.970	1.00	22.40
ATOM	2083 2084	o	PRO A		21.806	6.678	-2.613	1.00	24.00
MOTA MOTA	2085	CB	PRO A		18.961	6.900	-4.218	1.00	25.65
ATOM	2085	CG	PRO A		17.537	7.358	-4.127	1.00	26.81
ATOM	2087	CD	PRO F		17.721	8.776	-3.602	1.00	27.78
ATOM	2088	N	LYS F		21.468	8.722	-3.459	1.00	26.43
ATOM	2089	CA	LYS A		22.901	9.004	-3.540	1.00	26.72
MOTA	2090	C	LYS A	311	23.311	9.641	-2.232	1.00	24.76
ATOM	2091	0	LYS A	311	24.503	9.699	-1.918	1.00	24.86
MOTA	2092	CB	LYS A	A 311	23.260	9.885	-4.744	1.00	29.52
MOTA	2093	CG	LYS A	A 311	22.367	11.086	-4.950	1.00	32.23
MOTA	2094	CD	LYS A	A 311	22.797	11.902	-6.187	1.00	35.53 34.62
ATOM	2095	CE	LYS A	A 311	22.506	11.184	-7.503	1.00	33.92
MOTA	2096	NZ		A 311	21.041	11.064	-7.750	1.00	24.19
MOTA	2097	N		A 312	22.305	10.090	-1.467	1.00 1.00	22.42
MOTA	2098	CA		A 312	22.505	10.685	-0.137	1.00	22.08
MOTA	2099	С		A 312	22.626	9.531	0.856 1.724	1.00	22.80
MOTA	2100	0		A 312	23.504	9.532 11.563	0.253	1.00	18.83
MOTA	2101	CB		A 312	21.313		0.233		15.41
MOTA	2102	CG		A 312	21.589		0.492		12.74
MOTA	2103		1 LEU		20.376 22.791		0.944		13.01
ATOM	2104		2 LEU .		21.782		0.643		21.73
MOTA	2105	N		A 313	21.715		1.453		21.11
MOTA	2106			A 313 A 313	21.686				21.89
ATOM	2107			A 313	20.628				23.17
MOTA	2108			A 313	20.477				20.42
MOTA	2109 2110			A 313	20.457				21.54
MOTA	2111		1 PHE		19.446				21.51
MOTA MOTA	2112		2 PHE		21.471			1.00	18.24
ATOM	2113		1 PHE		19.451			1.00	23.36
MOTA	2114		2 PHE		21.497				20.28
MOTA	2115			A 313	20.485				19.77
MOTA	2116			A 314	22.862	5.608	0.104		22.26
ATOM	2117			A 314	23.081	4.437			27.78
ATOM	2118			A 314	22.453				29.90
ATOM	2119			A 314	22.210				29.70
MOTA	2120			A 314	24.599				28.60
MOTA	2121			A 314	25.054	5.722	-0.677	7 1.00	23.83

## FIG. 2KK

									24 26
MOTA	2122	CD P	RO A 314	ŀ	24.138	6.290	0.380	1.00	24.26 32.62
MOTA	2123		SP A 315		22.234	2.190	-1.059 -0.641	1.00	35.70
MOTA	2124		SP A 315		21.627	0.937	0.173	1.00	33.22
MOTA	2125		SP A 315		22.591	0.064 -0.826	0.173	1.00	32.53
MOTA	2126		SP A 315		22.176	0.194	-1.864	1.00	41.44
MOTA			SP A 315		21.080	-0.767	-1.504	1.00	47.92
MOTA			SP A 315		19.948 18.782	-0.303	-1.389	1.00	48.99
MOTA			SP A 31		20.228	-1.986	-1.335	1.00	50.65
MOTA			SP A 31		23.878	0.368	0.041	1.00	32.70
MOTA			ER A 31		24.945	-0.321	0.753	1.00	32.11
ATOM	2132		ER A 316		24.964	0.046	2.234	1.00	33.20
ATOM	2133		SER A 31		25.765	-0.494	3.008	1.00	33.99
MOTA	2134		SER A 31		26.296	0.025	0.116	1.00	33.15
MOTA	2135 2136		SER A 31		26.322	1.361	-0.365	1.00	32.59
MOTA	2137		LEU A 31		24.110	0.996	2.610	1.00	33.53
MOTA	2137		LEU A 31		23.996	1.446	3.993	1.00	33.28
ATOM ATOM	2139		LEU A 31		22.946	0.626	4.721	1.00	35.30
ATOM	2140		LEU A 31		23.066	0.385	5.917	1.00	37.21
MOTA	2141		LEU A 31		23.603	2.923	4.054	1.00	30.83
ATOM	2142		LEU A 31		24.645	3.949	3.619	1.00	29.13 26.44
ATOM	2143		LEU A 31		24.099	5.348	3.856	1.00	28.48
ATOM	2144	CD2	LEU A 31	17	25.933	3.718	4.399	1.00 1.00	36.65
ATOM	2145		PHE A 31		21.901	0.237	3.999	1.00	35.98
ATOM	2146		PHE A 31		20.817	-0.550	4.570 4.175	1.00	39.10
MOTA	2147		PHE A 31		21.016	-2.003	3.192	1.00	39.40
MOTA	2148		PHE A 31		21.696	-2.303 -0.135	4.030	1.00	32.24
MOTA	2149		PHE A 3		19.446	1.326	4.131	1.00	29.76
MOTA	2150		PHE A 3		19.156 19.675	2.211	3.192	1.00	30.03
MOTA	2151		PHE A 3		18.272	1.800	5.087	1.00	29.55
MOTA	2152	CD2	PHE A 3	10 10	19.320	3.562	3.191	1.00	30.88
MOTA	2153		PHE A 3		17.902	3.147	5.107	1.00	32.47
ATOM	2154 2155	CEZ	PHE A 3		18.423	4.038	4.147	1.00	29.56
MOTA	2156	N	PRO A 3		20.423	-2.923	4.950	1.00	41.02
ATOM ATOM	2157	CA	PRO A 3		20.469	-4.370	4.763	1.00	40.92
MOTA	2158	C	PRO A 3		19.664		3.523	1.00	40.26
ATOM	2159	Ō	PRO A 3		18.445		_		40.41 40.44
ATOM	2160	CB	PRO A 3	19	19.817		and the second s		38.98
ATOM	2161	CG	PRO A 3		20.171				42.72
ATOM	2162	CD	PRO A 3	19	19.834				39.10
ATOM	2163	N	ALA A 3		20.347				39.58
ATOM	2164	CA	ALA A 3		19.712				39.61
MOTA	2165	C	ALA A 3		19.866				41.72
MOTA	2166	0	ALA A 3		20.040				43.99
ATOM	2167		ALA A 3		20.320 19.806				36.36
MOTA	2168	N	ASP A 3		19.800				31.72
MOTA	2169		ASP A. 3		19.502	-10.243		_	29.16
MOTA	2170	_	ASP A 3		18 680	11.233	0.980		33.72
MOTA	2171		ASP A 3		20.638	-10.134	3.263	1.00	29.58
MOTA	2172		ASP A 3		20.024		L 4.575	1.00	26.63
MOTA	2173		ASP A :		18.840		9 4.624		28.64
MOTA	2174		ASP A :		20.757	7 -9.73	9 5.573		27.21
MOTA		_	SER A		17.57	L -9.72°	7 2.22		23.95
MOTA			SER A		16.29	5 -10.35	7 1.99		21.48
MOTA MOTA			SER A		15.286	6 -9.38			
ATOM			SER A		15.50	o -8.18			
MOTA			SER A		15.76		1 3.29	5 1.00	25.55



## FIG. 2LL

MOTA	2181	OG	SER A	A 322		15.11		-9.994	4.117	1.00	29.61
ATOM	2182	N	GLU A	A 323		14.16	8	-9.929	0.955	1.00	18.90
ATOM	2183	CA	GLU A	A 323		13.11	3	-9.134	0.376	1.00	20.38 -
MOTA	2184	С	GLU A	A 323		12.40		-8.299	1.424	1.00	20.46
MOTA	2185	0	GLU A	A 323		11.66		-7.373	1.091	1.00	21.68
ATOM	2186	CB	GLU A	A 323				10.034	-0.349	1.00	17.47
ATOM	2187	CG	GLU 2	A 323		12.71	.5 -	10.719	-1.559	1.00	24.16
ATOM	2188	CD		A 323		12.70		-9.861	-2.846	1.00	26.03
ATOM	2189		GLU Z			13.04	0 -	10.412	-3.926	1.00	28.72
ATOM	2190	OE2		A 323		12.35		-8.664	-2.789	1.00	23.50
ATOM	2191	N		A 324		12.58		-8.638	2.695	1.00	22.03
ATOM	2192	CA		A 324		11.95		-7.866	3.767	1.00	19.77
ATOM	2193	C		A 324		12.81		-6.631	4.016	1.00	15.64
ATOM	2194	0		A 324		12.33		-5.503	3.984	1.00	14.85
	2195	CB		A 324		11.83		-8.718	5.041	1.00	18.59
MOTA	2196	CG		A 324		11.42		-7.938	6.254	1.00	17.00
MOTA			HIS .			12.33		-7.349	7.106	1.00	15.47
MOTA	2197		HIS .			10.20		-7.651	6.762	1.00	16.90
ATOM	2198					11.69		-6.732	8.080	1.00	14.50
ATOM	2199		HIS.			10.39		-6.900	7.896	1.00	15.07
MOTA	2200		HIS			14.10		-6.864	4.196	1.00	15.06
ATOM	2201	N		A 325		15.04		-5.800	4.443	1.00	18.56
MOTA	2202	CA		A 325		15.1		-4.855	3.254	1.00	21.93
MOTA	2203	C		A 325				-3.719	3.414	1.00	26.00
ATOM	2204	0		A 325		15.63		-6.385	4.789	1.00	19.57
ATOM	2205	CB		A 325		16.43		-7.076	6.144	1.00	21.82
MOTA	2206	CG		A 325		16.43	_	-7.160	6.831	1.00	21.71
ATOM	2207		ASN			15.43		-7.569	6.535	1.00	17.20
MOTA	2208		ASN			17.6			2.053	1.00	21.92
ATOM	2209	N		A 326		14.8		-5.362	0.838	1.00	17.60
MOTA	2210	CA		A 320		14.9		-4.564	0.769	1.00	15.87
MOTA	2211	C		A 32		13.7		-3.685	0.769	1.00	15.12
MOTA	2212	0		A 32		13.7		-2.516	-0.392	1.00	18.74
MOTA	2213	CB		A 32		15.0		-5.462		1.00	19.18
MOTA	2214	CG		A 32		16.3		-6.142	-0.598		18.11
MOTA	2215	CD		A 32		16.2		-7.055	-1.796	1.00	19.55
ATOM	2216	CE		A 32		17.6		-7.461	-2.243	1.00	25.56
MOTA	2217	NZ		A 32		17.5		-8.481	-3.340	1.00	13.43
MOTA	2218	N		A 32		12.5		-4.248	1.145	1.00	14.62
MOTA	2219	CA		A 32		11.3		-3.501	1.145	1.00	17.67
MOTA	2220	C		A 32		11.3		-2.485	2.302	1.00	
MOTA	2221	0		A 32		10.7		-1.412	2.196	1.00	19.98
MOTA	2222	CB		A 32		10.1		-4.461	1.246	1.00	10.36
MOTA	2223	CG		A 32		8.7		-3.803	1.262	1.00	12.10
ATOM	2224	CDI		A 32		8.5		-2.894	0.021	1.00	15.96
ATOM	2225	CD2	LEU			7.7		-4.883	1.328	1.00	12.46
ATOM	2226	N		A 32		11.9	92	-2.820	3.396	1.00	17.49
ATOM	2227	CA		A 32		12.0		-1.932	4.542	1.00	16.76
MOTA	2228	C		A 32		13.0		-0.790	4.269		14.85
MOTA	2229	0		A 32		`12.8	06	0.361	4.647		15.55
MOTA	2230	CB	LYS	A 32	В	12.4	97	-2.723	5.784		13.97
ATOM	2231	CG	LYS	A 32	В	11.3	81	-3.476	6.440		12.37
ATOM	2232	CD		A 32		10.2	66	-2.520	6.773		15.62
ATOM	2233	CE		A 32		8.9	98	-3.236	7.124		18.22
ATOM	2234	NZ	LYS	A 32	8	7.9	28	-2.271			27.89
ATOM	2235	N	ALA	A 32	9	14.1		-1.131	3.596		11.88
MOTA	2236			A 32		15.1	.88	-0.194			13.33
ATOM	2237			A 32		14.6	96	0.924			14.85
MOTA	2238		ALA	A 32	9	15.2	270	2.010			11.99
ATOM	2239		ALA	A 32	9	16.3		-0.927	2.592	1.00	12.09
					•						

## FIG. 2MM

			~== *	220	-	13.663	0.621	1.559	1.00	16.65
ATOM	2240		SER A				1.568	0.647	1.00	20.24
MOTA	2241		SER A			13.046		1.430	1.00	19.37
MOTA	2242		SER A			12.014	2.374		1.00	20.59
MOTA	2243		SER F			11.680	3.503	1.075	1.00	19.48
MOTA	2244		SER P			12.361	0.820	-0.510		23.75
MOTA	2245	OG	SER P	7 330		11.717	1.714	-1.396	1.00	
MOTA	2246	N	GLN F	331		11.460	1.762	2.462	1.00	18.23
MOTA	2247	CA	GLN A	¥ 331		10.494	2.442	3.290	1.00	19.23
ATOM	2248	C	GLN A	A 331		11.219	3.484	4.124	1.00	19.62
ATOM	2249	0	GLN A	A 331	:	10.726	4.586	4.308	1.00	19.08
ATOM	2250	CB	GLN A	A 331		9.787	1.451	4.191	1.00	15.77
MOTA	2251	CG	GLN A	A 331		8.474	1.061	3.629	1.00	16.36
MOTA	2252	CD	GLN A	A 331		8.030	-0.292	4.087	1.00	14.43
ATOM	2253	OE1	GLN A	A 331		8.762	-0.994	4.763	1.00	23.19
ATOM	2254	NE2		A 331		6.829	-0.673	3.718	1.00	12.76
ATOM	2255	N		A 332		12.422	3.133	4.562	1.00	19.54
ATOM	2256	CA		A 332		13.249	3.994	5.384	1.00	19.46
ATOM	2257	C		A 332		13.761	5.205	4.623	1.00	21.75
	2258	ō		A 332		13.957	6.266	5.203	1.00	22.56
MOTA	2259	СВ		A 332		14.421	3.207	5.932	1.00	14.44
MOTA	2259	N		A 333		14.003	5.045	3.331	1.00	21.94
MOTA		CA		A 333		14.509	6.142	2.536	1.00	22.76
ATOM	2261	C		A 333		13.390	7.123	2.259	1.00	22.62
MOTA	2262					13.589	8.332	2.216	1.00	22.94
MOTA	2263	0		A 333		15.079	5.628	1.222	1.00	25.59
MOTA	2264	CB		A 333		16.450	6.149	0.922	1.00	26.01
MOTA	2265	CG		A 333			5.976	-0.524	1.00	25.64
ATOM	2266	CD		A 333		16.778	5.255	-0.680	1.00	32.29
MOTA	2267	NE		A 333		18.026	3.936	-0.831	1.00	35.86
MOTA	2268	CZ		A 333		18.108		-0.847	1.00	36.93
MOTA	2269			A 333		17.000	3.191		1.00	39.62
MOTA	2270	NH2		A 333		19.299	3.362	-0.992 2.128	1.00	20.64
MOTA	2271	N		A 334		12.191	6.594		1.00	21.35
MOTA	2272	CA		A 334		11.054	7.423	1.846	1.00	22.23
ATOM	2273	C		A 334		10.724	8.307	3.028		24.26
MOTA	2274	0		A 334		10.322	9.451	2.846	1.00	22.69
MOTA	2275	CB		A 334		9.867	6.547	1.526	1.00	21.51
MOTA	2276	CG		A 334		8.780	7.294	0.836	1.00	25.96
ATOM	2277			A 334		8.988	7.667	-0.344	1.00	
MOTA	2278	QD2	ASP	A 334		7.720	7.485	1.469	1.00	23.53
MOTA	2279	N		A 335		10.852	7.762	4.235	1.00	21.61
ATOM	2280	CA	LEU	A 335		10.564	8.522	5.441	1.00	19.50
ATOM	2281	C	LEU	A 335		11.643	9.582	5.571	1.00	18.55
ATOM	2282	0	LEU	A 335		11.348	10.746	5.840	1.00	17.43
ATOM	2283	CB	LEU	A 335		10.537	7.617	6.681	1.00	17.26
ATOM	2284	CG	LEU	A 335		10.015	8.264	7.977	1.00	16.18
MOTA	2285		LEU	A 335		8.588	8.746	7.786	1.00	16.01
MOTA	2286			A 335		10.076	7.276	9.131	1.00	14.68
ATOM	2287	N		A 336		12.887	9.179	5.336	1.00	16.64
ATOM	2288	CA		A 336		14.005	10.086	5.407	1.00	16.93
MOTA	2289	C		A 336		13.807	11.218	4.413	1.00	19.18
ATOM	2290	ō	LEU	A 336		14.043	12.382	4.736	1.00	24.01
ATOM	2291	СВ		A 336		15.299	9.358	5.071	1.00	14.09
ATOM	2291	CG		A 336		16.249		6.179	1.00	16.94
		CD1	ाज्ञा	A 336		17.503		5.565	1.00	10.16
ATOM	2293	CD	ווערנ כ	A 336		16.599		7.102	1.00	13.20
ATOM	2294		022	A 337		13.315		3.226	1.00	17.20
MOTA	2295	N		A 337		13.114		2.184	1.00	14.95
MOTA	2296	CA		A 337		12.032		2.559		13.10
ATOM	2297	C		A 337		12.090		2.158		15.70
MOTA	2298	0	SER	A 33/		.a. 090			_	

## FIG. 2NN

ATOM	2299	СВ	SER A	337	12.837	11.222	0.800	1.00	9.08
ATOM	2300	OG	SER A		11.455	11.067	0.520	1.00	6.87
ATOM	2301	N	LYS A		11.060	12.421	3.344	1.00	12.04
MOTA	2302	CA	LYS A		9.962	13.281	3.764	1.00	12.08
ATOM	2303	C	LYS A		10.242	14.118	5.032	1.00	14.69
ATOM	2304	ō	LYS A		9.586	15.131	5.295	1.00	11.13
ATOM	2305	CB	LYS A		8.733	12.429	3.990	1.00	12.09
MOTA	2306	CG	LYS A		8.203	11.758	2.763	1.00	12.08
ATOM	2307	CD	LYS A		7.002	10.919	3.111	1.00	12.89
ATOM	2308	CE	LYS A		6.220	10.601	1.882	1.00	20.87
MOTA	2309	NZ	LYS A		7.157	10.324	0.750	1.00	24.91
MOTA	2310	N	MET A		11.216	13.666	5.814	1.00	16.21
ATOM	2311	CA	MET A	339	11.600	14.310	7.046	1.00	16.11
ATOM	2312	C	MET A	339	12.691	15.354	6.832	1.00	16.02
MOTA	2313	O	MET A		12.602	16.458	7.374	1.00	17.20
ATOM	2314	CB	MET A	339	12.075	13.260	8.066	1.00	17.91
ATOM	2315	CG	MET A		11.016	12.221	8.487	1.00	15.40
MOTA	2316	SD	MET A	A 339	11.399	11.344	10.070	1.00	11.13
ATOM	2317	CE	MET A		9.803	10.977	10.535	1.00	4.76
ATOM	2318	N	LEU A		13.745	14.995	6.102	1.00	13.03
ATOM	2319	CA		A 340	14.815	15.942	5.847	1.00	9.12
ATOM	2320	С	LEU A	A 340	14.414	16.893	4.749	1.00	9.02
ATOM	2321	0	LEU 2	A 340	14.950	16.822	3.655	1.00	11.54
MOTA	2322	CB	LEU Z	A 340	16.112	15.232	5.464	1.00	10.00
MOTA	2323	CG	LEU 2	A 340	16.730	14.338	6.536	1.00	13.72
ATOM	2324	CD1	LEU 2	A 340	18.045	13.775	6.031	1.00	13.72
ATOM	2325	CD2	LEU .	A 340	16.945	15.144	7.815	1.00	12.06
MOTA	2326	N	VAL .	A 341	13.399	17.708	5.002	1.00	10.15
ATOM	2327	CA	VAL .	A 341	12.947	18.693	4.029		16.38
MOTA	2328	C	VAL .	A 341	13.129	20.074	4.642	1.00	18.38
MOTA	2329	0	VAL .	A 341	12.477	20.393	5.620	1.00	20.26
ATOM	2330	CB	VAL	A 341	11.472	18.547	3.681	1.00	15.80
MOTA	2331	CG1	VAL	A 341	11.198	19.269	2.396	1.00	12.46
MOTA	2332	CG2	VAL	A 341	11.086	17.106	3.565	1.00	21.60
MOTA	2333	N	ILE	A 342	13.968	20.909	4.040	1.00	21.30
ATOM	2334	CA	ILE	A 342	14.224	22.252	4.559	1.00	23.13
ATOM	2335	С	ILE	A 342	12.966	23.094	4.698	1.00	22.57
MOTA	2336	0	ILE	A 342	12.845	23.856	5.650	1.00	24.81
ATOM	2337	CB	ILE	A 342	15.260	23.013	3.704	1.00	24.58
MOTA	2338	CG1	LLE	A 342	16.591	22.252	3.691	1.00	21.38
MOTA	2339	CG2	ILE	A 342		24:473	4.213	1.00	28.32
MOTA	2340	CD1		A 342		22.857	2.776	1.00	21.55
MOTA	2341	N	ASP	A 343	12.004	22.931	3.801	1.00	20.64
MOTA	2342	CA		A 343	10.797	23.719	3.911	1.00	18.43
ATOM	2343	С	ASP	A 343			4.789	1.00	19.72
MOTA	2344	0		A 343			4.364	1.00	22.83
MOTA	2345	CB		A 343			2.514	1.00	19.98
MOTA	2346	CG	ASP	A 343			2.510	1.00	22.57
MOTA	2347			A 343			3.492	1.00	23.19
MOTA	2348	OD2	2 ASP	A 343	8.872		1.508	1.00	26.66
MOTA	2349	N		A 344			5.990		20.20
MOTA	2350	CA		A 344		23.018	6.894		16.72
MOTA	2351	C	PRO	A 344			6.304		18.97
MOTA	2352	0		A 344			6.854		19.62
MOTA	2353	CB	PRO	A 344			8.075		17.59
MOTA	2354	CG	PRO	A 344			7.461		17.94
MOTA	2355	CD	PRO	A 344			6.574		18.08
MOTA	2356	N	ALA	A 345	6.862		5.235		19.74
ATOM	2357	CA		A 345		23.694	4.548	1.00	18.23

## FIG. 200

MOTA	2358	C	ALA .	A 345		5.453	22.445	3.724	1.00	17.55
ATOM	2359	0	ALA .	A 345		4.350	22.043	3.381	1.00	19.09
ATOM	2360	CB	ALA.	A 345		5.458	24.927	3.659	1.00	18.19
MOTA	2361	N	LYS .	A 346		6.589	21.831	3.420	1.00	18.76
MOTA	2362	CA	LYS .	A 346		6.635	20.590	2.653	1.00	22.13
MOTA	2363	С	LYS .	A 346		7.160	19.356	3.444	1.00	22.18
MOTA	2364	0	LYS .	A 346		7.104	18.231	2.952	1.00	22.05
MOTA	2365	CB	LYS .	A 346		7.468	20.811	1.385	1.00	26.61
MOTA	2366	CG	LYS	A 346		6.903	21.904	0.471	1.00	33.55
MOTA	2367	CD	LYS .	A 346		7.743	22.051	-0.789	1.00	38.48
MOTA	2368	CE	LYS	A 346		7.883	20.707	-1.515	1.00	43.70
ATOM	2369	NZ	LYS	A 346		8.631	20.765	-2.819	1.00	47.82
ATOM	2370	N	ARG	A 347		7.648	19.575	4.664	1.00	19.68
ATOM	2371	CA	ARG	A 347		8.174	18.519	5.527	1.00	17.00
MOTA	2372	С	ARG	A 347		7.004	17.683	6.064	1.00	16.03
ATOM	2373	0	ARG	A 347		5.874	18.151	6.082	1.00	15.59
ATOM	2374	CB		A 347		8.956	19.158	6.678	1.00	16.04
ATOM	2375	CG		A 347		9.829	18.222	7.483	1.00	15.84
ATOM	2376	CD		A 347		10.449	18.926	8.675	1.00	16.35
ATOM	2377	NE		A 347		11.419	19.939	8.266	1.00	17.58
MOTA	2378	CZ	ARG	A 347		11.472	21.176	8.757	1.00	16.09
ATOM	2379			A 347		10.606	21.553	9.680	1.00	18.02
ATOM	2380			A 347	•	12.385	22.042	8.319	1.00	14.89
MOTA	2381	N	ILE	A 348		7.254	16.437	6.466	1.00	16.76
ATOM	2382	CA	ILE	A 348		6.180	15.575	6.984	1.00	16.86
ATOM	2383	C		A 348		5.909	15.867	8.466	1.00	17.05
ATOM	2384	Ō	ILE	A 348		6.805	16.319	9.180	1.00	18.30
ATOM	2385	СВ		A 348		6.484	14.031	6.734	1.00	18.03
MOTA	2386			A 348		5.235	13.195	6.988	1.00	19.19
MOTA	2387	CG2		A 348		7.610	13.523	7.608	1.00	12.85
ATOM	2388			A 348		5.455	11.731	6.750	1.00	22.05
MOTA	2389	N	SER	A 349		4.666	15.651	8.901	1.00	15.54
ATOM	2390	CA	SER	A 349		4.257	15.912	10.273	1.00	15.42
ATOM	2391	С	SER	A 349		4.443	14.695	11.187	1.00	18.21
MOTA	2392	0	SER	A 349		4.959	13.665	10.748	1.00	19.66
ATOM	2393	CB	SER	A 349		2.808	16.395	10.297	1.00	13.74
ATOM	2394	OG	SER	A 349		1.896	15.362	9.984	1.00	15.03
MOTA	2395	N	VAL	A 350		4.047	14.821	12.460	1.00	20.51
ATOM	2396	CA	VAL	A 350		4.198	13.738	13.447	1.00	18.94
ATOM	2397	C	VAL	A 350		3.147	12.664	13.230	1.00	16.49
MOTA	2398	0	VAL	A 350		3.446	11.478	13.336	1.00	18.02
ATOM	2399	CB	VAL	A 350		4.083	14.250	14.941	1.00	19.83
ATOM	2400	CG1	VAL	A 350		4.553	13.183	15.922	1.00	14.18
MOTA	2401	CG2	VAL	A 350		4.893	15.506	15.153	1.00	19.35
ATOM	2402	N	ASP	A 351		1.928	13.087	12.912	1.00	15.82
ATOM	2403	CA		A 351		0.821	12.167	12.696	1.00	19.48
ATOM	2404	C		A 351		0.886	11.383	11.404	1.00	21.44
ATOM	2405	ō		A 351		0.288	10.322	11.289	1.00	24.24
ATOM	2406	CB		A 351		-0.517	12.896	12.802	1.00	19.34
MOTA	2407	CG		A 351		-0.818	13.346	14.216	1.00	22.25
MOTA	2408			A 351		-1.880	13.959	14.447	1.00	21.31
ATOM	2409			A 351		0.014	13.083	15.108	1.00	23.43
ATOM	2410	N		A 352		1.568	11.922	10.409	1.00	21.74
ATOM	2411	CA		A 352		1.699	11.221	9.152	1.00	20.56
ATOM	2412	C		A 352		2.953	10.380	9.214	1.00	19.06
MOTA	2413	ō		A 352		3.059	9.378	8.516	1.00	20.14
ATOM	2414	СВ		A 352		1.797	12.191	7.967	1.00	21.74
MOTA	2415	CG		A 352		0.504	12.922	7.680	1.00	20.06
ATOM	2416			A 352		-0.591	12.512	8.148	1.00	19.05
. = =										

## FIG. 2PP

ATOM	2417	OD2	ASP	Α	352		0.597	13.925	6.961	1.00	21.55
MOTA	2418	N.	ALA				3.925	10.819	10.002	1.00	16.38
MOTA	2419	CA	ALA	Α	353		5.154	10.082	10.141	1.00	15.27
MOTA	2420	C	ALA	A	353		4.845	8.814	10.954	1.00	18.82
ATOM	2421	0	ALA	Α	353		5.497	7.791	10.778	1.00	20.49
MOTA	2422	CB	ALA	A	353		6.240	10.943	10.789	1.00	9.63
MOTA	2423	N	LEU	А	354		3.791	8.854	11.766	1.00	19.59
ATOM	2424	CA	LEU	A	354		3.397	7.699	12.567	1.00	20.91
MOTA	2425	С	LEU	A	354		2.625	6.687	11.738	1.00	22.39
ATOM	2426	0	LEU				2.633	5.487	12.044	1.00	22.66
ATOM	2427	CB	LEU				2.581	8.144	13.782	1.00	20.28
MOTA	2428	CG	LEU				3.366	8.623	15.027	1.00	22.16
MOTA	2429		LEU				2.518	9.564	15.886	1.00	18.21 18.64
MOTA	2430		LEU				3.837	7.427	15.847	1.00	25.01
ATOM	2431	N	GLN				1.974	7.189	10.682	1.00	24.82
MOTA	2432	CA	GLN				1.193	6.385	9.732	1.00 1.00	24.02
MOTA	2433	,C	GLN				1.964	6.083	8.427	1.00	23.85
MOTA	2434	0	GLN				1.387	5.761	7.391 9.446	1.00	26.02
MOTA	2435	CB	GLN				-0.165	7.040	10.653	1.00	31.50
MOTA	2436	CG	_		355		-1.104	7.110	11.190	1.00	37.67
MOTA	2437	CD			355		-1.522	5.738	11.130	1.00	41.39
ATOM	2438		GLN			•	-0.731	4.777 5.654	11.670	1.00	41.86
MOTA	2439		GLN				-2.758	6.231	8.494	1.00	24.42
MOTA	2440	N			356		3.283		7.385	1.00	22.45
ATOM	2441	CA			356		4.169	5.916 4.424	7.609	1.00	24.49
ATOM	2442	C			356		4.396	3.996	8.729	1.00	24.40
ATOM	2443	0			356		4.648		7.550	1.00	18.90
MOTA	2444	CB			356		5.504	6.643 6.466	6.397	1.00	19.41
ATOM	2445	CG			356		6.447 6.368	7.226	5.249	1.00	17.71
ATOM	2446		HIS					5.665	6.243	1.00	16.97
MOTA	2447		HIS				7.524 7.359	6.902	4.439	1.00	13.61
ATOM	2448		HIS				8.075	5.960	5.020	1.00	17.38
ATOM	2449		HIS		357		4.337	3.619	6.544	1.00	25.58
ATOM	2450	N			357		4.538	2.170	6.656	1.00	22.18
ATOM	2451	CA			357		5.804	1.715	7.393	1.00	19.11
MOTA	2452	C			357		5.829	0.608	7.939	1.00	23.70
MOTA	2453				357		4.542	1.711	5.187	1.00	23.59
ATOM	2454	CB			357		4.997	2.946	4.429	1.00	23.68
ATOM	2455	CD			357		4.204	4.025	5.136	1.00	24.01
ATOM ATOM	2456 2457	N			358		6.855	2.523	7.407	1.00	13.73
ATOM	2457	CA			358		8.066	2.108	8.086	1.00	10.20
MOTA	2459	C			358		7.921	2.208	9.627	1.00	15.75
ATOM	2460	0			358		8.742	1.650	10.365	1.00	14.80
MOTA	2461	СВ			358		9.233	2.964	7.622	1.00	6.07
MOTA	2462	CG			358		10.577		8.168	1.00	6.30
MOTA	2463		TYR				11.287		7.563	1.00	8.94
ATOM	2464		TYR				11.151		9.282	1.00	8.80
ATOM	2465		L TYR				12.534		8.043	1.00	9.47
ATOM	2466	CE			358		12.409		9.773	1.00	8.25
ATOM	2467				358		13.094		9.144	1.00	5.06
ATOM	2468	OH			358		14.339		9.583	1.00	4.74
ATOM	2469		ILE	7	359		6.863			1.00	15.98
ATOM	2470	CA			359		6.613		11.511	1.00	16.40
ATOM	2471				359		5.243		12.004	1.00	18.15
ATOM	2472				359		5.088				24.14
ATOM	2473				359		6.714				15.03
ATOM	2474		l ILE				8.015				11.94
ATOM	2475		2 ILE				6.567			1.00	11.43
	-1.5			_							

# FIG. 2QQ

MOTA	2476	CD1	ILE .	A.	359	9.18	33	4.972	12.216	1.00	12.83
MOTA	2477	N	ASN .	A.	360	4.24		2.632	11.136	1.00	19.28
MOTA	2478	CA	ASN .	A	360	2.93		2.249	11.601	1.00	21.24
MOTA	2479	C	ASN .			2.80		0.778	12.026	1.00	19.53
ATOM	2480	0	ASN .			1.89		0.391	12.691	1.00	21.14
MOTA	2481	CB	ASN .			1.79		2.659	10.602	1.00	24.74
MOTA	2482	CG	ASN .			1.63		1.685	9.438	1.00	28.99
MOTA	2483		ASN .			2.63		1.150	8.913	1.00	34.08
MOTA	2484	ND2	ASN			0.39		1.473	9.016	1.00	28.15
ATOM	2485	N	VAL			3.80		0.033	11.702	1.00	18.76
MOTA	2486	CA	VAL			3.7		1.434	12.112	1.00	23.04
MOTA	2487	C	VAL			3.7		1.557	13.641	1.00	26.35
ATOM	2488	0	VAL			3.1		2.523	14.171	1.00	29.64
MOTA	2489	CB	VAL			4.9		2.258	11.594	1.00	19.01
MOTA	2490	CG1	VAL	Α	361	5.0		2.250	10.067	1.00	20.77
MOTA	2491	CG2	VAL			6.2		1.751	12.205	1.00	18.11
ATOM	2492	N	TRP			4.2		0.561	14.342	1.00	28.15
MOTA	2493	CA	TRP			4.3		0.541	15.811	1.00	24.02
MOTA	2494	C	TRP			3.2		0.314	16.440	1.00	22.25
MOTA	2495	0	TRP			3.1		0.352	17.650	1.00	28.38
MOTA	2496	CB	TRP			5.6		0.060	16.272	1.00	19.04
MOTA	2497	CG	TRP			6.8		-0.610	15.778	1.00	19.63
MOTA	2498		TRP			7.7		-0.128	14.872	1.00	21.93
MOTA	2499	CD2				7.3		-1.829	16.281	1.00	21.65
ATOM	2500	NE1				8.7		-0.961	14.801	1.00	21.62
MOTA	2501	CE2				8.5		-2.014	15.659	1.00	22.35
ATOM	2502	CE3				6.9		-2.769	17.206	1.00	20.16
MOTA	2503	CZ2				9.4		-3.113	15.957	1.00	20.95
MOTA	2504	CZ3				7.7		-3.841	17.498	1.00	16.39
MOTA	2505	CH2				8.9		-4.010	16.880	1.00	15.82 22.86
MOTA	2506	N	TYR			2.4		1.003	15.627	1.00	24.69
MOTA	2507	CA	TYR			1.4		1.910	16.095	1.00 1.00	28.12
MOTA	2508	C			363	0.4		1.297	17.097		30.75
MOTA	2509	0			363	0.1		0.134	16.954	1.00 1.00	26.24
MOTA	2510	CB			363	0.7		2.489	14.892	1.00	26.24
MOTA	2511	CG			363	-0.3		3.529	15.234	1.00	26.14
MOTA	2512	CD1			363	-1.6		3.188	15.408	1.00	28.71
MOTA	2513	CD2			363	0.0		4.856	15.405	1.00	27.93
MOTA	2514	CE1			363	-2.5		4.129	15.740	1.00	26.78
ATOM	2515	CE2			363	-0.8		5.809	15.744	1.00	25.74
MOTA	2516	CZ			363	-2.1		5.432	15.905 16.213	1.00	33.01
MOTA	2517	OH			363	-3.1		6.353	18.074	1.00	28.98
MOTA	2518	N			364	0.0		2.115		1.00	26.46
ATOM	2519	CA			364	-0.8		1.718 2.952	19.152 19.654	1.00	26.25
ATOM	2520	C			364	-1.5			20.160	1.00	29.14
ATOM	2521	0			364	-0.9		3.880	20.100	1.00	24.81
ATOM	2522	CB			364	-0.0		1.089 0.569	21.439	1.00	27.58
ATOM	2523	CG			364	-0.8			21.541	1.00	28.14
MOTA	2524		ASP			-2.0		0.932	22.268	1.00	34.84
ATOM	2525		ASP			-0.3			19.534		25.78
ATOM	2526	N			365	-2.8		2.968	20.000	1.00	28.64
ATOM	2527	CA			365	-3.6		4.119 4.580	20.000		30.94
ATOM	2528	C			365	-3.3			21.408		33.56
ATOM	2529	0			365	-2.8		5.690 3.641	19.849		27.83
MOTA	2530	CB			365	-5.0			18.555		27.49
MOTA	2531	CG			365	-5.0 -3.7		2.875 2.049	18.773		28.07
MOTA	2532	CD			. 365 . 366	-3.7		3.725	22.406		33.50
ATOM	2533	N				-3.2		4.086	23.802		34.17
MOTA	2534	CA	АЦА	A	366	-3.2	74	4.000	43.002		



## FIG. 2RR

								7 00	24 07
MOTA	2535	C	ALA A 366		-1.828	4.610	23.995 24.792	1.00 1.00	34.01 33.18
MOTA	2536	0	ALA A 366		-1.583	5.519 2.885	24.792	1.00	38.15
MOTA	2537	CB	ALA A 366		-3.490		23.215	1.00	34.87
ATOM	2538	N	GLU A 367		-0.913	4.046 4.384	23.223	1.00	35.12
MOTA	2539	CA	GLU A 367		0.508	5.663	22.429	1.00	36.01
ATOM	2540	С	GLU A 367		0.799	6.286	22.597	1.00	34.03
MOTA	2541	0	GLU A 367		1.846	3.229	22.607	1.00	36.74
MOTA	2542	CB	GLU A 367		1.283	2.921	23.231	1.00	37.45
MOTA	2543	CG	GLU A 367		2.622	1.742	22.543	1.00	37.93
MOTA	2544	CD	GLU A 367		3.323	1.476	21.340	1.00	34.38
ATOM	2545		GLU A 367		3.056	1.478	23.206	1.00	38.70
MOTA	2546	OE2	GLU A 367		4.148 -0.136	6.058	21.572	1.00	37.78
ATOM	2547	N	VAL A 368		0.034	7.262	20.774	1.00	38.83
MOTA	2548	CA	VAL A 368		-0.925	8.387	21.186	1.00	39.06
ATOM	2549	C	VAL A 368		-0.473	9.434	21.642	1.00	41.85
MOTA	2550	0	VAL A 368		-0.473	6.978	19.243	1.00	37.06
MOTA	2551	CB	VAL A 368		-0.058	8.277	18.463	1.00	37.21
MOTA	2552		VAL A 368		1.072	6.123	18.786	1.00	35.19
MOTA	2553	CG2			-2.233	8.197	21.011	1.00	40.22
MOTA	2554	N	GLU A 369		-2.233	9.241	21.377	1.00	42.42
MOTA	2555	CA	GLU A 369		-3.193	9.073	22.753	1.00	42.83
MOTA	2556	C	GLU A 369		-4.960	8.673	22.915	1.00	42.26
ATOM	2557	0	GLU A 369		-4.294	9.438	20.319	1.00	44.75
ATOM	2558	CB	GLU A 369		-5.014	8.180	19.855	1.00	45.12
MOTA	2559	CG	GLU A 369		-4.439	7.620	18.561	1.00	46.29
MOTA	2560	CD	GLU A 369 GLU A 369		-3.313	8.031	18.196	1.00	44.38
MOTA	2561				-5.115	6.774	17.922	1.00	44.39
ATOM	2562	OE2			-3.113	9.494	23.731	1.00	44.29
ATOM	2563	N	ALA A 370 ALA A 370		-3.378	9.420	25.126	1.00	45.80
ATOM	2564	CA	ALA A 370		-3.316	10.812	25.750	1.00	46.17
ATOM	2565	C	ALA A 370		-2.472	11.639	25.373	1.00	44.23
MOTA	2566	O	ALA A 370		-2.430	8.464	25.860	1.00	47.56
ATOM	2567	CB N	PRO A 371		-4.234	11.086	26.695	1.00	47.08
MOTA	2568	CA	PRO A 371		-4.333	12.370	27.412	1.00	47.97
ATOM	2569 2570	C	PRO A 371		-3.001	12.746	28.091	1.00	47.33
MOTA	2570 2571	Ö	PRO A 371		-2.308	11.887	28.651	1.00	48.84
MOTA	2572	СВ	PRO A 371		-5.446	12.091	28.438	1.00	47.47
ATOM	2572	CG	PRO A 371		-6.343	11.117	27.704	1.00	46.69
ATOM	2574	CD	PRO A 371		-5.312	10.173	27.119	1.00	46.13
MOTA MOTA	2575	N	PRO A 372		-2.584	14.030	27.959	1.00	44.53
ATOM	2576	CA	PRO A 372		-1.351	14.560	28.557	1.00	43.72
ATOM	2577	C	PRO A 372		-1.247	14.823	30.092	1.00	43.15
ATOM	2578	ō	PRO A 372		-0.392	14.225	30.755	1.00	38.33
MOTA	2579	СВ	PRO A 372		-1.060	15.805	27.692	1.00	42.06
ATOM	2580	CG			-2.418	16.198	27.182	1.00	43.54
MOTA	2581	CD	PRO A 372		-3.031	14.874	26.844	1.00	41.44
MOTA	2582	N	PRO A 373		-2.124	15.680	30.688	1.00	45.40
ATOM	2583	CA			-1.991	15.905	32.142	1.00	48.11
ATOM	2584	C	PRO A 373		-2.838	14.972	33.035		48.84
ATOM	2585	ō	PRO A 373		-3.957	15.358	33.472		47.99
ATOM	2586	СВ			-2.406	17.394	32.305		48.09
ATOM	2587	CG			-2.950	17.835	30.926		45.71
ATOM	2588	CD			-3.203	16.528	30.171		46.49
ATOM	2589		ALA A 379		5.622	28.512			42.15
MOTA	2590				4.671	27.944			45.12
ATOM	2591		ALA A 379		5.052	28.375	33.747		47.76
MOTA	2592		ALA A 379		5.397	27.528			47.42
ATOM	2593	-			3.230	28.364	35.511	1.00	42.23
			1	•					



# FIG. 2SS

						5.012	29.690	33.494	1.00	48.53
MOTA	2594	N	LEU A			5.343	30.273	32.190	1.00	46.22
ATOM	2595	CA	LEU A				30.312	32.046	1.00	48.02
MOTA	2596	C	LEU A			6.861		32.662	1.00	47.82
ATOM	2597	0	PEA :			7.522	31.138		1.00	43.91
MOTA	2598	CB	LEU 2			4.761	31.685	32.081		41.45
MOTA	2599	CG	LEU .			3.255	31.846	31.837	1.00	
MOTA	2600	CD1	LEU .	A 3	880	2.852	31.153	30.529	1.00	43.02
MOTA	2601	CD2	LEU .	A 3	880	2.464	31.288	32.988	1.00	37.93
MOTA	2602	N	ASP .	A 3	881	7.398	29.437	31.194	1.00	51.88
MOTA	2603	CA	ASP .	A 3	881	8.853	29.317	31.012	1.00	53.94
MOTA	2604	С	ASP .	A 3	881	9.538	29.929	29.770	1.00	54.51
ATOM	2605	0	ASP	A 3	381 <sup>°</sup>	10.041	29.214	28.892	1.00	53.90
MOTA	2606	CB	ASP	A 3	881	9.263	27.839	31.152	1.00	57.15
ATOM	2607	CG	ASP	A 3	381	8.520	27.109	32.277	1.00	58.25
ATOM	2608		ASP	A :	381	8.731	27.455	33.464	1.00	61.41
ATOM	2609		ASP			7.735	26.177	31.974	1.00	54.54
MOTA	2610	N	ALA			9.616	31.254	29.747	1.00	54.88
ATOM	2611	CA	ALA			10.269	32.050	28.702	1.00	53.46
	2612	C	ALA			10.336	33.434	29.382	1.00	54.54
MOTA		0	ALA			10.287	34.510	28.755	1.00	53.71
ATOM	2613		ALA			9.405	32.084	27.459	1.00	55.53
MOTA	2614	CB				10.481	33.331	30.700	1.00	52.53
MOTA	2615	N	ARG			10.518	34.404	31.679	1.00	48.12
MOTA	2616	CA	ARG			11.868	35.088	31.895	1.00	45.65
MOTA	2617	C	ARG				34.867	31.135	1.00	43.32
MOTA	2618	0_	ARG			12.817	33.784	32.991	1.00	48.15
MOTA	2619	CB	ARG			10.037		33.300	1.00	47.01
MOTA	2620	CG	ARG			10.757	32.453	34.099	1.00	45.98
MOTA	2621	CD	ARG			9.897	31.495		1.00	46.34
MOTA	2622	NE	ARG			9.381	32.145	35.294	1.00	45.23
MOTA	2623	$\mathbf{cz}$	ARG			8.271	31.795	35.935	1.00	46.97
MOTA	2624		ARG			7.531	30.776	35.516		45.75
ATOM	2625	NH2	ARG			7.863	32.517	36.969	1.00	43.73
MOTA	2626	N	GLU			11.908	35.937	32.932	1.00	
MOTA	2627	CA	GLU			13.102	36.688	33.357	1.00	41.03
ATOM	2628	C	GLU	Α	384	13.135	36.865	34.895	1.00	
MOTA	2629	0	GLU	A	384	12.148	37.306	35.505	1.00	34.88
ATOM	2630	CB	GLU	Α	384	13.102	38.080	32.742	1.00	45.48
ATOM	2631	CG	GLU	Α	384	12.783	38.134	31.257	1.00	49.70
MOTA	2632	CD	GLU	Α	384	12.403	39.535	30.785	1.00	50.64
ATOM	2633	OE1	GLU	Α	384	11.756	40.279	31.567	1.00	47.57
MOTA	2634	OE2	GLU	Α	384	12.746	39.874	29.625	1.00	53.02
ATOM	2635	N	HIS	A	385	14.273	36.521	35.504	1.00	34.45
ATOM	2636	CA	HIS	Α	385	14.468	36.644	36.950	1.00	30.28
ATOM	2637	C	HIS			15.931	36.683	37.261	1.00	28.54
MOTA	2638	ō	HIS			16.776	36.326	36.445	1.00	24.90
ATOM		СВ	HIS			13.917	35.454	37.737	1.00	27.07
ATOM	2640	CG	HIS			12.457	35.211	37.565	1.00	26.81
ATOM	2641		. HIS			11.504	35.855	38.314	1.00	27.05
ATOM	2642		HIS			11.790	34.342	36.766	1.00	28.23
ATOM	2643		HIS			10.304	35.396	37.990	1.00	31.75
			HIS			10.452	34.475	37.053	1.00	30.36
MOTA	2644				386	16.226		38.468		32.82
ATOM	2645	N			386	17.602				35.29
ATOM	2646	CA			386	17.002		39.623		33.04
MOTA	2647	C				17.071				30.47
MOTA	2648	0			386	17.880				37.45
MOTA	2649	CB			386	19.164				43.91
ATOM	2650	OG			386					36.33
MOTA	2651		2 THR			16.801				31.86
MOTA	2652	N	ILE	Α	387	19.257	33.044	37.023	2.00	22.00



#### FIG. 2TT

										•
MOTA	2653	CA	ILE 2	A	387	19.776	34.421	40.423	1.00	33.58
MOTA	2654	C	ILE 2			19.300	34.068	41.830	1.00	33.37
MOTA	2655	0	ILE 2			19.481	32.932	42.285	1.00	31.92
ATOM	2656	CB	ILE			21.315	34.393	40.388	1.00	35.68 33.18
MOTA	2657		ILE A			21.903	35.487	41.286	1.00	35.10
MOTA	2658		ILE A			21.789	34.535	38.940	1.00	29.75
MOTA	2659	CD1				23.412	35.408	41.424	1.00 1.00	33.15
ATOM	2660	N	GLU .			18.756	35.049	42.545 43.873	1.00	30.07
ATOM	2661	CA	GLU .			18.247 16.758	34.784 34.593	43.744	1.00	28.18
MOTA	2662	C	GLU .			16.736	33.879	44.518	1.00	26.25
MOTA	2663 2664	O CB	GLU .			18.650	35.897	44.828	1.00	35.56
ATOM ATOM	2665	CG	GLU .			20.174	35.911	45.063	1.00	42.10
ATOM	2666	CD	GLU .			20.759	34.510	45.329	1.00	45.57
MOTA	2667		GLU .			20.380	33.900	46.358	1.00	49.57
ATOM	2668		GLU			21.599	34.017	44.521	1.00	49.11
ATOM	2669	N	GLU .			16.202	35.192	42.708	1.00	25.49
ATOM	2670	CA	GLU .	Α	389	14.795	34.998	42.442	1.00	25.44
ATOM	2671	С	GLU	A	389	14.595	33.610	41.785	1.00	23.41
MOTA	2672	0	GLU			13.521	33.006	41.896	1.00	22.43
MOTA	2673	CB	GLU			14.270	36.103	41.549	1.00	27.39
MOTA	2674	CG	GLU			13.547	37.123	42.355	1.00	31.98 37.60
MOTA	2675	CD	GLU			12.863	38.134 37.982	41.501 41.322	1.00 1.00	40.54
ATOM	2676		GLU			11.630 13.547	37.962	41.024	1.00	36.37
MOTA	2677	OE2	TRP			15.640	33.113	41.124	1.00	18.95
MOTA	2678 2679	N CA	TRP			15.605	31.808	40.491	1.00	17.65
ATOM ATOM	2680	C	TRP			15.715	30.735	41.576	1.00	17.48
ATOM	2681	ō	TRP			14.966	29.767	41.597	1.00	19.35
ATOM	2682	CB	TRP			16.772	31.673	39.516	1.00	15.00
ATOM	2683	CG	TRP	Α	390	16.485	32.149	38.147	1.00	12.48
MOTA	2684	CD1	TRP	A	390	17.300	32.923	37.376	1.00	13.71
MOTA	2685	CD2	TRP	A	390	15.310	31.882	37.357	1.00	11.84
ATOM	2686	NE1				16.706	33.166	36.157	1.00	13.62
MOTA	2687		TRP			15.485	32.538	36.118	1.00 1.00	11.97 14.72
MOTA	2688	CE3				14.142	31.151 32.486	37.569 35.104	1.00	11.62
MOTA	2689	CZ2 CZ3	TRP TRP			14.529 13.186	31.099	36.553	1.00	14.87
MOTA	2690	CH2				13.386	31.759	35.338	1.00	11.15
MOTA MOTA	2691 2692	N N	LYS			16.651	30.941	42.490	1.00	20.23
ATOM	2693	CA	LYS			16.888	30.049	43.607	1.00	20.65
ATOM	2694	C	LYS			15.601	29.802	44.400	1.00	22.95
ATOM	2695	ō	LYS			15.301	28.654	44.748	1.00	24.92
ATOM	2696	СВ	LYS	Α	391	17.988	30.651	44.471	1.00	21.29
MOTA	2697	CG	LYS	A	391	18.444	29.831	45.640	1.00	20.35
MOTA	2698	CD	LYS	A	391	19.809	30.312	46.095	1.00	20.38
MOTA	2699	CE			391	20.072	29.882	47.532	1.00	24.61
ATOM	2700	NZ			391	21.393	30.332	48.051	1.00	26.71
MOTA	2701	N			392	14.824	30.849	44.682	1.00	22.91 23.21
ATOM	2702	CA			392	13.567	30.648	45.412	1.00 1.00	23.21
MOTA	2703	C			392	12.548 11.810	29.870 29.039	44.599 45.135		24.12
ATOM	2704	O			392 392	12.926	31.967	45.133	1.00	23.58
ATOM ATOM	2705 2706	CB			392	11.470	31.792	46.377		27.62
ATOM	2706	CD			392	11.219	32.416	47.762	1.00	30.72
MOTA	2707	OE1			392	12.080	33.184	48.243		34.21
ATOM	2709	OE2			392	10.157	32.158	48.370		30.26
MOTA	2710	N			393	12.436	30.212	43.322		22.69
MOTA	2711	CA	LEU	A	393	11.498	29.527	42.450	1.00	19.67



#### FIG. 2UU

MOTA	2712	С	PEA			11.862	28.036	42.415	1.00	16.28
ATOM	2713	0	LEU			11.010	27.163	42.580	1.00	16.68
ATOM	2714	CB	LEU			11.600	30.104	41.040	1.00	16.32
MOTA	2715	CG	LEU	A	393	10.942	31.443	40.796	1.00	11.54
MOTA	2716	CD1	LEU	Α	393	11.522	32.077	39.540	1.00	11.13
MOTA	2717	CD2	LEU	Α	393	9.453	31.217	40.635	1.00	12.66
ATOM	2718	N	ILE	Α	394	13.148	27.771	42.261	1.00	14.10
ATOM	2719	CA	ILE	Α	394	13.672	26.430	42.174	1.00	18.89
ATOM	2720	С			394	13.479	25.615	43.449	1.00	24.26
ATOM	2721	0			394	12.862	24.540	43.426	1.00	23.76
MOTA	2722	CB			394	15.140	26.499	41.738	1.00	17.71
ATOM	2723	CG1	ILE			15.191	26.982	40.280	1.00	17.72
ATOM	2724	CG2	ILE			15.835	25.173	41.915	1.00	20.38
ATOM	2725	CD1			394	16.539	26.785	39.598	1.00	17.90
ATOM	2726	N	TYR			13.974	26.145	44.567	1.00	26.90
ATOM	2727	CA	TYR			13.845	25.497	45.868	1.00	27.68
ATOM	2728	C	TYR			12.365	25.241	46.140	1.00	29.10
ATOM	2729	o	TYR			11.984	24.213	46.697	1.00	30.47
ATOM	2723	СВ	TYR			14.426	26.414	46.943	1.00	26.11
ATOM	2731	CG	TYR				25.831	48.330	1.00	23.85
	2732	CD1	TYR			14.492				
ATOM						15.527	24.995	48.701	1.00	20.88
MOTA	2733	CD2	TYR			13.568	26.186	49.292	1.00	25.32
ATOM	2734	CE1	TYR			15.648	24.530	49.993	1.00	25.62
MOTA	2735	CE2	TYR			13.680	25.728	50.609	1.00	28.23
ATOM	2736	CZ	TYR			14.717	24.906	50.950	1.00	27.68
MOTA	2737	OH	TYR			14.814	24.469	52.245	1.00	33.57
MOTA	2738	N	LYS			11.524	26.166	45.697	1.00	31.19
MOTA	2739	CA	LYS			10.089	26.072	45.874	1.00	29.83
ATOM	2740	C	LYS			9.520	24.805	45.222	1.00	29.47
ATOM	2741	0	LYS			8.622	24.168	45.783	1.00	31.87
ATOM	2742	CB	LYS			9.451	27.297	45.236	1.00	31.22
ATOM	2743	CG	LYS			8.555	28.104	46.129	1.00	34.16
MOTA	2744	CD	LYS			9.323	28.880	47.193	1.00	36.62
MOTA	2745	CE	LYS			8.449	29.995	47.763	1.00	36.94
MOTA	2746	NZ	LYS	Α	396	8.227	31.096	46.745	1.00	38.25
ATOM	2747	N	GLU	Α	397	10.012	24.458	44.030	1.00	26.39
ATOM	2748	CA	GLU	A	397	9.524	23.280	43.308	1.00	23.47
ATOM	2749	C	GLU	Α	397	10.077	21.984	43.863	1.00	19.67
ATOM	2750	0	GLU	Α	397	9.398	20.968	43.869	1.00	18.33
ATOM	2751	CB	GLU	Α	397	9.851	23.372	41.806	1.00	27.02
MOTA	2752	CG	GLU	A	397	8.703	23.869	40.887	1.00	27.93
MOTA	2753	CD	GLU	Α	397	7.601	22.839	40.651	1.00	27.60
MOTA	2754	OE1	GLU	Α	397	7.891	21.632	40.652	1.00	26.85
MOTA	2755	OE2	GLU	A	397	6.433	23.233	40.451	1.00	30.96
ATOM	2756	N	VAL	A	398	11.332	22.003	44.276	1.00	19.84
ATOM	2757	CA	VAL			11.966	20.822	44.833	1.00	23.53
ATOM	2758	С	VAL	Α	398	11.255	20.413	46.119	1.00	26.29
ATOM	2759	0	VAL			11.114	19.217	46.400	1.00	29.23
ATOM	. 2760	CB	VAL			13.466	21.068	45.127	1.00	23.54
ATOM	2761		VAL			14.140	19.801	45.608	1.00	18.61
ATOM	2762	CG2				14.157	21.618	43.883	1.00	25.50
ATOM	2763	N	MET			10.789	21.404	46.884	1.00	28.85
ATOM	2764	CA	MET			10.081	21.137	48.135	1.00	31.54
ATOM	2765	C	MET			8.612	20.924	47.867	1.00	34.05
ATOM	2766	ō	MET			7.892	20.478	48.753	1.00	36.36
ATOM	2767	CB	MET			10.242	22.287	49.129	1.00	29.76
ATOM	2768	CG	MET			11.666	22.576	49.515	1.00	32.50
ATOM	2769	SD	MET			12.612	21.136	50.101	1.00	34.26
ATOM	2770	CE	MET			12.505	21.419	51.848	1.00	42.05
<b></b>				-1	ررر	_2.505		52.040		5



## FIG. 2VV

MOTA	2771	N	ASN A 400	8.185	21.209	46.636	1.00	38.05
ATOM	2772	CA	ASN A 400	6.782	21.075	46.197	1.00	42.57
ATOM	2773	C	ASN A 400	5.706	20.912	47.262	1.00	44.57
MOTA	2774	0	ASN A 400	4.935	21.885	47.424	1.00	46.32
MOTA	2775	CB	ASN A 400	6.585	20.032	45.047	1.00	44.49
MOTA	2776	CG	ASN A 400	7.320	18.689	45.274	1.00	46.24
ATOM	2777	OD1	ASN A 400	6.968	17.908	46.161	1.00	46.77
MOTA	2778	ND2	ASN A 400	8.289	18.390	44.401	1.00	44.05
ATOM	2779	C5	5184A1001	21.681	10.532	31.356	1.00	27.28
MOTA	2780	C6	5184A1001	22.457	11.213	30.225	1.00	28.05
MOTA	2781	01	5184A1001	23.279	10.622	29.499	1.00	24.49
MOTA	2782	N1	5184A1001	22.218	12.549	30.129	1.00	26.81
MOTA	2783	C2	5184A1001	21.369	13.245	30.873	1.00	25.98
MOTA	2784	из	5184A1001	20.662	12.674	31.791	1.00	28.30
ATOM	2785	C4	5184A1001	20.874	11.283	32.149	1.00	25.17
MOTA	2786	02	5184A1001	21.212	14.442	30.751	1.00	28.54
MOTA	2787	C11	5184A1001	21.776	9.055	31.557	1.00	28.26
MOTA	2788	04	5184A1001	21.021	8.534	32.380	1.00	29.45
MOTA	2789	N4	5184A1001	22.670	8.379	30.822	1.00	28.04
MOTA	2790	C1	5184A1001	23.707	4.452	30.694	1.00	24.51
MOTA	2791	C12	5184A1001	24.236	5.340	29.725	1.00	24.47
MOTA	2792	C3	5184A1001	23.837	6.674	29.834	1.00	25.42
MOTA	2793	C14	5184A1001	22.957	7.050	30.868	1.00	25.69
MOTA	2794	C7	5184A1001	22.454	6.120	31.816	1.00	25.22
MOTA	2795	C9	5184 <b>A1</b> 001	22.836	4.784	31.730	1.00	20.54
MOTA	2796	N2	5184A1001	20.058	10.764	33.215	1.00	24.72
MOTA	2797	C16	5184A1001	18.674	11.516	36.553	1.00	14.97
MOTA	2798	C13	5184A1001	19.542	11.079	35.546	1.00	19.43
ATOM	2799	C17	5184A1001	19.290	11.368	34.202	1.00	23.47
ATOM	2800	C15	5184A1001,	18.143	12.127	33.889	1.00	25.12
MOTA	2801	C8	5184A1001	17.248	12.570	34.935	1.00	24.24
ATOM	2802	C10	5184A1001	17.543	12.248	36.274	1.00	15.35
MOTA	2803	OH2	TIP3B 1	19.519	6.665	33.090	1.00	11.81
ATOM	2804	OH2	TIP3B 2	14.148	22.210	28.179	1.00	20.00
MOTA	2805	OH2	TIP3B 3	16.487	15.191	32.609	1.00	20.00
				END				



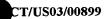
FIG. 3A

	Atom	Туре	e Resid	<u>#</u>		<u>x</u>	<u>¥</u>	<u>z</u>	<u>Occ</u>	<u>B</u>
ATOM	1	СВ	ASP	45	:	19.290	11.912	62.876	1.00	82.67
ATOM	2	CG	ASP	45	:	20.511	12.303	63.724	1.00	82.67
MOTA	3	OD1	ASP	45		21.632	12.419	63.162	1.00	82.67
ATOM	4	OD2	ASP	45		20.347	12.500	64.956	1.00	82.67
ATOM	5	C	ASP	45		19.675	12.871	60.534	1.00	40.50 82.67
ATOM	6	0	ASP	45		19.435	13.632	59.587	1.00 1.00	40.50
MOTA	7	N	ASP	45		17.424	12.934	61.581 61.859	1.00	40.50
MOTA	8	CA	ASP	45		18.894	13.005 11.939	60.468	1.00	17.90
MOTA	9	N	ASN	46		20.618 21.385	11.740	59.249	1.00	17.90
ATOM	10	CA	ASN	46 46		22.723	11.074	59.552	1.00	34.81
ATOM	11	CB CG	ASN ASN	46		23.710	12.021	60.171	1.00	34.81
MOTA	12 13		ASN	46		23.339	13.104	60.639	1.00	34.81
MOTA	14		ASN	46		24.976	11.627	60.190	1.00	34.81
ATOM ATOM	15	C	ASN	46		20.650	10.894	58.227	1.00	17.90
ATOM	16	õ	ASN	46		20.826	9.675	58.195	1.00	34.81
MOTA	17	N	GLN	47		19.813	11.534	57.410	1.00	2.36
ATOM	18	CA	GLN	47		19.079	10.827	56.360	1.00	2.36
ATOM	19	СВ	GLN	47		17.776	11.552	55.999	1.00	25.20
ATOM	20	CG	GLN	47		16.591	11.308	56.965	1.00	25.20
MOTA	21	CD	GLN	47		15.309	12.062	56.565	1.00	25.20
MOTA	22	OE1	GLN	47		14.200	11.509	56.578	1.00	25.20
ATOM	23	NE2	GLN	47		15.462	13.338	56.226	1.00	25.20
ATOM	24	C	GLN	47		20.005	10.791	55.149	1.00	2.36 25.20
MOTA	25	0	GLN	47		19.903	9.907	54.306	1.00	25.20
MOTA	26	N	PHE	48		20.976	11.704	55.137	1.00 1.00	2.00
MOTA	27	CA	PHE	48		21.929	11.832	54.040 53.588	1.00	2.00
MOTA	28	CB	PHE	48		22.025	13.288	53.274	1.00	2.00
MOTA	29	CG	PHE	48		20.701	13.893 14.404	54.296	1.00	2.00
ATOM	30		PHE	48		19.915 20.197	13.869	51.976	1.00	2.00
MOTA	31		PHE	48		18.638	14.876	54.054	1.00	2.00
ATOM	32		PHE	48 48		18.918	14.337	51.707	1.00	2.00
ATOM	33	CE2	PHE PHE	48		18.128	14.845	52.760	1.00	2.00
MOTA MOTA	34 35	C	PHE	48		23.314	11.359	54.369	1.00	2.00
ATOM	36	Ö	PHE	48		23.672	11.164	55.529	1.00	2.00
ATOM	37	N	TYR	49		24.098	11.171	53.320	1.00	2.00
ATOM	38	CA	TYR	49		25.465	10.754	53.478	1.00	2.00
ATOM	39	CB	TYR	49		25.572	9.230	53.557		7.42
MOTA	40	CG	TYR	49		25.519	8.504	52.242	1.00	7.42
ATOM	41		1 TYR	49		24.305	8.195	51.643	1.00	7.42
ATOM	42		l TYR	49		24.255	7.486			7.42 7.42
ATOM	43		2 TYR	49		26.684		51.619		7.42
MOTA	44		2 TYR	49		26.641				7.42
ATOM	45			49		25.426				7.42
ATOM	46			49		25.387				2.00
ATOM	47		TYR	49		26.250 25.746				7.42
ATOM	48		TYR	49		27.484		_		12.70
MOTA	49		SER	50 50		28.346				12.70
ATOM	50 51			50		29.144				44.73
ATOM	52 52			50		28.278				44.73
MOTA	52 53		SER	50		29.303				12.70
MOTA MOTA	53 54		SER	50		29.989				44.73
ATOM	55		VAL	51		29.343				12.81
ATOM	56			51		30.238				12.81
MOTA	57			51		29.531			1.00	2.00



# FIG. 3B

MOTA	58	CG1	VAL	51	28.521	9.154	47.453	1.00	2.00
MOTA	59	CG2	VAL	51	30.557	7.887	48.125	1.00	2.00
ATOM	60	C	VAL	51	30.898	10.933	47.828	1.00	12.81
ATOM	61	0	VAL	51	30.242	11.660	47.076	1.00	2.00
MOTA	62	N	GLU	52	32.222	10.801	47.753	1.00	26.73
ATOM	63	CA	GLU	52	33.013	11.448	46.709	1.00	26.73
MOTA	64	CB	GLU	52	34.479	11.575	47.151	1.00	23.83
ATOM	65	CG	GLU	52	35.286	12.607	46.355	1.00	23.83
ATOM	66	CD	GLU	52	34.838	14.037	46.631	1.00	23.83
MOTA	67	OE1	GLU	52	34.719	14.388	47.824	1.00	23.83
ATOM	68	OE2	GLU	52	34.605	14.804	45.666	1.00	23.83
MOTA	69	C	GLU	52	32.921	10.677	45.388	1.00	26.73
ATOM	70	0	GLU	52	33.710	9.760	45.127	1.00	23.83 31.39
MOTA	71	N	VAL	53	31.948	11.054	44.562	1.00	31.39
MOTA	72	CA	VAL	53	31.741	10.409	43.266	1.00	19.10
MOTA	73	CB	VAL	53	30.228	10.287	42.885	1.00	19.10
MOTA	74		VAL	53	30.072	9.701	41.480	1.00	19.10
MOTA	75		VAL	53	29.496	9.401	43.878	1.00	
MOTA	76	C	VAL	53	32.471	11.190	42.175	1.00	31.39 19.10
MOTA	77	0	VAL	53	32.073	12.305	41.814	1.00	28.22
MOTA	78	N	GLY	54	33.554	10.603	41.670	1.00	28.22
ATOM	79	CA	GLY	54	34.329	11.234	40.617	1.00	28.22
MOTA	80	C	GLY	54	35.125	12.430	41.089	1.00	37.37
MOTA	81	0	GLY	<b>54</b>	36.150	12.291	41.758	1.00	24.29
ATOM	82	N	ASP	55	34.617	13.611	40.767	1.00 1.00	24.29
MOTA	83	CA	ASP	<b>55</b>	35.257	14.881	41.106 39.784	1.00	45.10
MOTA	84	CB	ASP	55 	35.557	15.616		1.00	45.10
MOTA	85	CG	ASP	55	36.481	16.802	39.952 40.524	1.00	45.10
ATOM	86		ASP	55	37.585	16.632	39.466	1.00	45.10
MOTA	87		ASP	55	36.110	17.895	41.969	1.00	24.29
MOTA	88	C	ASP	55	34.317	15.730 16.829	42.404	1.00	45.10
ATOM	89	0	ASP	55	34.669	15.193	42.214	1.00	28.43
MOTA	90	N	SER	56 56	33.126	15.876	42.974	1.00	28.43
MOTA	91	CA	SER	56	32.089	16.086	42.060	1.00	50.26
ATOM	92	CB	SER	56 56	30.865 30.177	17.303	42.334	1.00	50.26
ATOM	93	OG	SER	56 56	31.686	15.067	44.207	1.00	28.43
MOTA	94	C	SER	56 56	31.861	13.852	44.254	1.00	50.26
ATOM	95	0	SER	56 57	31.159	15.751	45.213	1.00	21.09
ATOM	96	N	THR THR	57 57	30.724	15.085	46.428	1.00	21.09
MOTA	97	CA	THR	5 <i>7</i> 57	31.153	15.856	47.683	1.00	27.49
ATOM	98 99	CB OG1		5 <i>7</i> 57	32.532	16.234	47.561	1.00	27.49
ATOM	100	CG2		57	30.967	14.991	48.931	1.00	27.49
MOTA		C	THR	57	29.208	14.955	46.444	1.00	21.09
ATOM	101 102	Ö	THR	57 57	28.498	15.934	46.680	1.00	27.49
MOTA	102	N	PHE	58	28.721	13.749	46.173	1.00	33.68
MOTA	103	CA	PHE	58	27.290	13.494	46.171	1.00	33.68
ATOM ATOM	105	CB	PHE	58	26.942	12.309	45.281	1.00	8.44
	105	CG	PHE	58	26.690	12.677	43.841	1.00	8.44
ATOM ATOM	107		PHE	58	27.731	13.123	43.030	1.00	8.44
ATOM	108		PHE	58	25.425	12.514	43.286	1.00	8.44
ATOM	109		PHE	58	27.526	13.382	41.671	1.00	8.44
ATOM	110	CE2		58	25.198	12.765	41.930	1.00	8.44
ATOM	111	CZ	PHE	58	26.252	13.207	41.119	1.00	8.44
ATOM	112	C	PHE	58	26.790	13.230	47.584	1.00	33.68
ATOM	113	o	PHE	58	27.306	12.360	48.283	1.00	8.44
ATOM	114	N	THR		25.836	14.045	48.017	1.00	2.00
ATOM	115	CA	THR		25.235	13.913	49.331	1.00	2.00
ATOM	116		THR		25.238	15.234	50.117	1.00	2.11
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## FIG. 3C

ATOM	117	OG1	THR	59	26.579	15.724	50.239	1.00	2.11
MOTA	118	CG2	THR	59	24.658	15.016	51.488	1.00	2.11
ATOM	119	С	THR	59	23.803	13.478	49.095	1.00	2.00
MOTA	120	0	THR	59	22.910	14.290	48.899	1.00	2.11
MOTA	121	N	VAL	60	23.598	12.174	49.091	1.00	16.21
MOTA	122	CA	VAL	60	22.281	11.629	48.857	1.00	16.21
MOTA	123	CB	VAL	60	22.316	10.642	47.669	1.00	12.96
ATOM	124	CG1	VAL	60	22.576	11.384	46.380	1.00	12.96
MOTA	125	CG2	VAL	60	23.409	9.597	47.883	1.00	12.96
MOTA	126	C	VAL	60	21.700	10.933	50.078	1.00	16.21
ATOM	127	0	VAL	60	22.367	10.773	51.098	1.00	12.96
MOTA	128	N	LEU	61	20.423	10.577	49.964	1.00	2.00
ATOM	129	CA	LEU	61	19.689	9.868	51.001	1.00	2.00
ATOM	130	CB	LEU	61	18.228	9.724	50.591	1.00	19.79
ATOM	131	CG	LEU	61	17.323	10.947	50.539	1.00	19.79
ATOM	132	CD1	LEU	61	16.195	10.678	49.580	1.00	19.79
ATOM	133	CD2	LEU	61	16.787	11.243	51.919	1.00	19.79
MOTA	134	С	LEU	61	20.271	8.471	51.136	1.00	2.00
ATOM	135	0	LEU	61	20.721	7.889	50.163	1.00	19.79
ATOM	136	N	LYS	62	20.179	7.903	52.328	1.00	37.57
ATOM	137	CA	LYS	62	20.713	6.567	52.597	1.00	37.57
MOTA	138	СВ	LYS	62	20.514	6.215	54.080	1.00	12.42
ATOM	139	CG	LYS	62	21.129	7.196	55.073	1.00	12.42
ATOM	140	CD	LYS	62	22.637	7.031	55.239	1.00	12.42
ATOM	141	CE	LYS	62	23.193	8.033	56.258	1.00	12.42
ATOM	142	NZ	LYS	62	22.571	7.914	57.624	1.00	12.42
ATOM	143	C	LYS	62	20.184	5.431	51.708	1.00	37.57
	144	o	LYS	62	20.898	4.467	51.448	1.00	12.42
ATOM ATOM	145	N	ARG	63	18.942	5.543	51.250	1.00	5.93
ATOM	146	CA	ARG	63	18.334	4.516	50.406	1.00	5.93
	147	CB	ARG	63	16.890	4.912	50.057	1.00	2.00
ATOM	148	CG	ARG	63	16.779	6.198	49.253	1.00	2.00
ATOM		CD	ARG	63	15.381	6.764	49.236	1.00	2.00
MOTA	149 150	NE	ARG	63	14.458	5.942	48.467	1.00	2.00
ATOM		CZ	ARG	63	13.205	6.281	48.192	1.00	2.00
ATOM	151		L ARG	63	12.718	7.423	48.625	1.00	2.00
MOTA	152		ARG	63	12.428	5.465	47.500	1.00	2.00
ATOM	153	C	ARG	63	19.140	4.295	49.129	1.00	5.93
ATOM	154		ARG	63	19.239	3.168	48.640	1.00	2.00
ATOM	155	0		64	19.715	5.384	48.615	1.00	12.13
MOTA	156	N	TYR TYR	64	20.516	5.377	47.391	1.00	12.13
MOTA	157	CA	TYR	64	20.460	6.764	46.721	1.00	2.00
ATOM	158	CB CG	TYR	64	19.066	7.169	46.288	1.00	2.00
ATOM	159	CD		64	18.358	6.407	45.361	1.00	2.00
MOTA	160			64	17.052	6.724	45.011	1.00	2.00
ATOM	161		1 TYR	64	18.422	8.275	46.844	1.00	2.00
MOTA	162		2 TYR		17.109	8.599	46.487	1.00	2.00
ATOM	163	CE:		64 64	16.432	7.810	45.571	1.00	2.00
ATOM	164		TYR			8.058	45.230	1.00	2.00
MOTA	165			64	15.118 21.951	4.968	47.710	1.00	12.13
ATOM	166		TYR	64			48.360		2.00
ATOM	167		TYR	64 65	22.691	5.711	47.242		2.00
MOTA	168		GLN	65 65	22.349				2.00
ATOM	169			65	23.675				32.87
MOTA	170			65	23.582				32.87
MOTA	171			65 65	22.537				32.87
MOTA	172			65	21.813				32.87
ATOM	173		1 GLN	65 65	21.091				32.87
MOTA	174		2 GLN	65	21.990				2.00
ATOM	175	C	GLN	65	24.468	2.770	46.347	1.00	4.00

#### FIG. 3D

MOTA	176	0	GLN	65	23.912	2.442	45.298	1.00	32.87
MOTA	177	N	ASN	66	25.783	2.677	46.550	1.00	28.78
MOTA	178	CA	ASN	66	26.745	2.207	45.561	1.00	28.78
MOTA	179	CB	ASN	66	26.528	0.746	45.218	1.00	23.20
MOTA	180	CG	ASN	66	27.649	0.186	44.374	1.00	23.20
ATOM	181	OD1	ASN	66	27.409	-0.590	43.449	1.00	23.20
ATOM	182	ND2	ASN	66	28.879	0.591	44.668	1.00	23.20
MOTA	183	С	ASN	66	26.680	3.054	44.319	1.00	28.78
ATOM	184	0	ASN	66	26.403	2.566	43.225	1.00	23.20
ATOM	185	N	<b>LEU</b>	67	26.961	4.335	44.514	1.00	28.28
MOTA	186	CA	LEU	67	26.928	5.310	43.442	1.00	28.28
MOTA	187	CB	LEU	67	27.105	6.717	44.014	1.00	5.06
MOTA	188	CG	LEU	67	26.056	7.332	44.932	1.00	5.06
ATOM	189		LEU	67	25.803	8.741	44.446	1.00	5.06
MOTA	190	CD2	LEU	67	24.758	6.538	44.949	1.00	5.06
MOTA	191	C	LEU	67	28.000	5.065	42.389	1.00	28.28
MOTA	192	0	<b>TE</b> U	67	29.169	4.878	42.717	1.00	5.06
MOTA	193	N	LYS	68	27.584	4.986	41.134	1.00	4.06
MOTA	194	CA	LYS	68	28.520	4.828	40.029	1.00	4.06
MOTA	195	CB	LYS	68	28.249	3.541	39.233	1.00	30.89
ATOM	196	CG	LYS	68	28.684	2.239	39.906	1.00	30.89
MOTA	197	CD	LYS	68	27.651	1.114	39.714	1.00	30.89
ATOM	198	CE	LYS	68	27.352	0.852	38.225	1.00	30.89
MOTA	199	NZ	LYS	68	26.455	-0.335	37.986	1.00	30.89
MOTA	200	С	LYS	68	28.269	6.044	39.143	1.00	4.06
ATOM	201	0	LYS	68	27.130	6.316	38.761	1.00	30.89
MOTA	202	N	PRO	69	29.319	6.841	38.874	1.00	44.94
MOTA	203	CD	PRO	69	30.714	6.698	39.337	1.00	33.19 44.94
MOTA	204	CA	PRO	69	29.156	8.027	38.023	1.00	33.19
ATOM	205	CB	PRO	69	30.492	8.752	38.196	1.00	33.19
ATOM	206	CG	PRO	69	31.475	7.618	38.394	1.00	44.94
MOTA	207	C	PRO	69	28.925	7.587	36.576	1.00	33.19
MOTA	208	0	PRO	69	29.574	6.657	36.090	1.00	11.68
ATOM	209	N	ILE	70	27.943	8.198	35.922	1.00	11.68
ATOM	210	CA	ILE	70	27.612	7.848	34.544	1.00 1.00	15.82
MOTA	211	CB	ILE	70	26.421	6.854	34.506	1.00	15.82
MOTA	212	CG2		70	26.794	5.535	35.192	1.00	15.82
ATOM	213		ILE	70	25.222	7.453	35.236 34.955	1.00	15.82
MOTA	214	CD1		70	23.924	6.747 9.078	33.713	1.00	11.68
MOTA	215	C	ILE	70	27.230		32.837	1.00	15.82
ATOM	216	0	ILE	70	26.365	8.989 10.214	33.959	1.00	53.07
MOTA	217	N	GLY	71	27.884		33.218	1.00	53.07
MOTA	218	CA	GLY	71	27.544	11.425		1.00	53.07
ATOM	219	C	GLY	71	28.586	12.527	33.070 32.147	1.00	47.75
MOTA	220	0	GLY	71	29.419	12.471	33.938	1.00	33.54
MOTA	221	N	SER	72	28.502	13.543	33.924	1.00	33.54
ATOM	222	CA	SER	72	29.400	14.711 14.285	33.924	1.00	47.06
ATOM	223	CB	SER	72	30.878	14.205	34.997	1.00	47.06
ATOM	224	OG	SER	72	31.592	15.607	32.716	1.00	33.54
ATOM	225	C	SER	72	29.135 28.349	16.563	32.710	1.00	47.06
ATOM	226	O	SER	72		15.379	37.733	1.00	14.51
ATOM	227	CB	ILE	77 77	27.336 28.188	14.104	37.638	1.00	14.51
MOTA	228	CG2		77 77		16.653	37.434	1.00	14.51
MOTA	229		LILE	77 77	28.142	16.653	38.389	1.00	14.51
MOTA	230		LILE	77 22	29.294	14.058	37.115	1.00	32.22
MOTA	231	C	ILE	77 77	25.290		38.207	1.00	14.51
ATOM	232	0	ILE	77 77	24.717	13.978	36.838	1.00	32.22
MOTA	233	N	ILE	77 77	25.299	16.530	36.771	1.00	32.22
MOTA	234	CA	ILE	77	26.134	15.291	55.771	1.00	J



#### FIG. 3E

									0.00
ATOM	235	N	VAL	78	25.197	13.114	36.177	1.00	2.00
MOTA	236	CA	VAL	78	24.407	11.907	36.396	1.00	2.00
MOTA	237	CB	VAL	78	23.839	11.313	35.083	1.00	6.06
ATOM	238	CG1	VAL	78	22.756	10.284	35.408	1.00	6.06
ATOM	239	CG2	VAL	78	23.279	12.411	34.177	1.00	6.06
MOTA	240	C	VAL	78	25.198	10.845	37.133	1.00	2.00
ATOM	241	0	VAL	78	26.419	10.736	36.983	1.00	6.06
ATOM	242	N	CYS	79	24.484	10.048	37.918	1.00	14.03
ATOM	243	CA	CYS	79	25.112	9.016	38.713	1.00	14.03
ATOM	244	CB	CYS	79	25.565	9.636	40.024	1.00	23.50
	245	SG	CYS	79	26.799	8.691	40.861	1.00	23.50
ATOM		C	CYS	79	24.178	7.836	38.975	1.00	14.03
ATOM	246			79 79	23.128	7.996	39.581	1.00	23.50
ATOM	247	0	CYS		24.578	6.649	38.524	1.00	14.88
ATOM	248	N	ALA	80			38.707	1.00	14.88
MOTA	249	CA	ALA	80	23.782	5.438			19.57
MOTA	250	СВ	ALA	80	24.281	4.360	37.783	1.00	
MOTA	251	C	ALA	80	23.831	4.956	40.147	1.00	14.88
MOTA	252	0	ALA	80	24.850	5.100	40.820	1.00	19.57
ATOM	253	N	ALA	81	22.728	4.401	40.634	1.00	5.14
ATOM	254	CA	ALA	81	22.703	3.909	42.005	1.00	5.14
ATOM	255	CB	ALA	81	22.560	5.055	42.962	1.00	20.04
ATOM	256	C	ALA	81	21.593	2.916	42.246	1.00	5.14
ATOM	257	0	ALA	81	20.689	2.771	41.425	1.00	20.04
MOTA	258	N	TYR	82	21.676	2.227	43.382	1.00	10.44
ATOM	259	CA	TYR	82	20.672	1.251	43.787	1.00	10.44
ATOM	260	CB	TYR	82	21.365	0.005	44.330	1.00	17.29
ATOM	261	CG	TYR	82	20.477	-0.907	45.132	1.00	17.29
			TYR	82	19.335	-1.475	44.572	1.00	17.29
ATOM	262			82	18.509	-2.330	45.311	1.00	17.29
MOTA	263	CE1			20.780	-1.212	46.450	1.00	17.29
MOTA	264	CD2		82			47.197	1.00	17.29
ATOM	265	CE2		82	19.964	-2.069			17.29
ATOM	266	CZ	TYR	82	18.832	-2.623	46.619	1.00	17.29
MOTA	267	OH	TYR	82	18.049	-3.479	47.351	1.00	
ATOM	268	С	TYR	82	19.763	1.830	44.861	1.00	10.44
ATOM	269	0	TYR	82	20.246	2.290	45.885	1.00	17.29
MOTA	270	N	ASP	83	18.457	1.830	44.623	1.00	5.91
MOTA	271	CA	ASP	83	17.525	2.325	45.624	1.00	5.91
ATOM	272	CB	ASP	83	16.299	2.969	44.989	1.00	26.75
ATOM	273	CG	ASP	83	15.358	3.573	46.021	1.00	26.75
ATOM	274	OD1	ASP	83	15.707	3.588	47.211	1.00	26.75
ATOM	275		ASP	83	14.269	4.050	45.656	1.00	26.75
ATOM	276	C	ASP	83	17.088	1.131	46.466	1.00	5.91
ATOM	277	ō	ASP	83	16.418	0.217	45.972	1.00	26.75
	278	N	ALA	84	17.415	1.181	47.755	1.00	3.12
ATOM	279	CA	ALA	84	17.099	0.113	48.680	1.00	3.12
ATOM		CB	ALA	84	17.949	0.249	49.920	1.00	15.64
ATOM	280				15.626	0.049	49.043	1.00	3.12
MOTA	281	C	ALA	84		-1.025	49.355	1.00	15.64
MOTA	282	0	ALA	84	15.123			1.00	2.05
MOTA	283	N	VAL	85	14.923	1.176	48.979		2.05
ATOM	284	CA	VAL	85	13.503	1.203	49.320	1.00	
ATOM	285	CB	VAL	85	13.012	2.652	49.634	1.00	2.17
ATOM	286		VAL	85	11.487	2.690	49.830	1.00	2.17
MOTA	287	CG2	VAL	85	13.718	3.172	50.883	1.00	2.17
ATOM	288	C	VAL	85	12.625	0.586	48.243	1.00	2.05
ATOM	289	0	VAL	85	11.834	-0.321	48.510	1.00	2.17
ATOM	290	N	LEU	86	12.784	1.094	47.026	1.00	6.01
ATOM	291	CA	LEU	86	12.030	0.649	45.859	1.00	6.01
ATOM	292	CB	LEU	86	12.116	1.726	44.784	1.00	19.18
ATOM	293	CG	LEU	86	10.838	2.271	44.158	1.00	19.18
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## FIG. 3F

ATOM	294	CD1	LEU	86	9.901	2.763	45.248	1.00	19.18
ATOM	295	CD2		86	11.203	3.392	43.186	1.00	19.18
ATOM	296	C	LEU	86	12.585	-0.655	45.307	1.00	6.01
ATOM	297	Ō	LEU	86	11.890	-1.369	44.591	1.00	19.18
ATOM	298	N	ASP	87	13.837	-0.948	45.649	1.00	2.44
ATOM	299	CA	ASP	87	14.539	-2.147	45.199	1.00	2.44
	300	CB	ASP	87	13.928	-3.445	45.782	1.00	23.73
MOTA		CG	ASP	87	14.691	-4.710	45.341	1.00	23.73
MOTA	301		ASP	87	15.932	-4.794	45.560	1.00	23.73
ATOM	302				14.045	-5.612	44.751	1.00	23.73
ATOM	303		ASP	87		-2.228	43.674	1.00	2.44
MOTA	304	C	ASP	87	14.650	-3.071	43.017	1.00	23.73
ATOM	305	0	ASP	87	14.020		43.130	1.00	6.10
MOTA	306	N	ARG	88	15.468	-1.339			6.10
MOTA	307	CA	ARG	88	15.734	-1.260	41.700	1.00	
MOTA	308	CB	ARG	88	14.490	-0.823	40.902	1.00	16.86
MOTA	309	CG	ARG	88	13.796	0.433	41.398	1.00	16.86
ATOM	310	CD	ARG	88	12.410	0.571	40.797	1.00	16.86
MOTA	311	NE	ARG	88	12.349	1.547	39.706	1.00	16.86
ATOM	312	$\mathbf{C}\mathbf{Z}$	ARG	88	11.238	2.182	39.327	1.00	16.86
MOTA	313	NH1	ARG	88	10.089	1.943	39.956	1.00	16.86
MOTA	314		ARG	88	11.263	3.057	38.326	1.00	16.86
ATOM	315	C	ARG	88	16.845	-0.258	41.537	1.00	6.10
ATOM	316	Ö	ARG	88	17.301	0.340	42.512	1.00	16.86
ATOM	317	N	ASN	89	17.315	-0.100	40.311	1.00	21.92
MOTA	318	CA	ASN	89	18.378	0.848	40.067	1.00	21.92
		CB	ASN	89	19.448	0.232	39.178	1.00	6.92
ATOM	319	CG	ASN	89	20.210	-0.864	39.884	1.00	6.92
MOTA	320				21.057	-0.588	40.718	1.00	6.92
ATOM	321	OD1		89	19.891	-2.114	39.578	1.00	6.92
ATOM	322		ASN	89	17.821	2.144	39.510	1.00	21.92
MOTA	323	C	ASN	89		2.156	38.782	1.00	6.92
MOTA	324	0	ASN	89	16.824		39.950	1.00	2.00
MOTA	325	N	VAL	90	18.433	3.237		1.00	2.00
MOTA	326	CA	VAL	90	18.044	4.579	39.567		2.00
MOTA	327	CB	VAL	90	17.273	5.295	40.721	1.00	
MOTA	328	CG1		90	15.944	4.612	40.995	1.00	2.00
MOTA	329	CG2	VAL	90	18.112	5.324	41.985	1.00	2.00
MOTA	330	С	VAL	90	19.246	5.441	39.153	1.00	2.00
ATOM	331	0	VAL	90	20.409	5.041	39.299	1.00	2.00
ATOM	332	N	ALA	91	18.935	6.609	38.590	1.00	2.00
ATOM	333	CA	ALA	91	19.920	7.584	38.140	1.00	2.00
MOTA	334	CB	ALA	91	19.749	7.871	36.659	1.00	2.00
ATOM	335	C	ALA	. 91	19.680	8.844	38.952	1.00	2.00
ATOM	336	0	ALA	91	18.565	9.335	39.027	1.00	2.00
ATOM	337	N	ILE	92	20.731	9.343	39.583	1.00	12.92
ATOM	338	CA	ILE	92	20.646	10.544	40.401	1.00	12.92
MOTA	339	CB	ILE	92	21.263	10.298	41.817	1.00	2.00
MOTA	340		2 ILE	92	21.166	11.566	42.671	1.00	2.00
ATOM	341		LILE	92	20.583	9.100	42.502	1.00	2.00
		CD:		92	21.274	8.619	43.742	1.00	2.00
ATOM	342				21.397	11.673	39.702	1.00	12.92
MOTA	343	C	ILE	92		11.534	39.361	1.00	2.00
MOTA	344		ILE	92	22.570		39.539	1.00	9.99
MOTA	345		LYS	93	20.726	12.803			9.99
MOTA	346			93	21.313	13.946	38.870	1.00	
MOTA	347			93	20.419	14.349	37.697	1.00	19.91
MOTA	348			93	20.968	15.445	36.831	1.00	19.91
ATOM	349			93	19.986	15.786	35.748		19.91
ATOM	350	CE	LYS	93	20.615		34.704		19.91
MOTA	351			93	19.611	16.999	33.658		19.91
MOTA	352		LYS	93	21.506	15.130	39.817	1.00	9.99
		_							

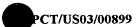


FIG. 3G

		_					40 200	1 00	10 01
MOTA	353	0	LYS	93	20.538	15.702	40.322	1.00	19.91
ATOM	354	N	LYS	94	22.763	15.491	40.056	1.00	7.04
ATOM	355	ÇA	LYS	94	23.086	16.609	40.931	1.00	7.04
ATOM	356	CB	LYS	94	24.434	16.381	41.605	1.00	2.00
ATOM	357	CG	LYS	94	24.823	17.501	42.548	1.00	2.00
ATOM	358	CD	LYS	94	26.242	17.356	43.019	1.00	2.00
				94	26.594	18.461	43.976	1.00	2.00
ATOM	359	CE	LYS					1.00	2.00
ATOM	360	NZ	LYS	94	27.975	18.303	44.477		
MOTA	361	С	LYS	94	23.138	17.944	40.191	1.00	7.04
MOTA	362	0	LYS	94	24.036	18.167	39.374	1.00	2.00
MOTA	363	N	LEU	95	22.197	18.834	40.503	1.00	2.00
MOTA	364	CA	LEU	95	22.129	20.168	39.913	1.00	2.00
ATOM	365	CB	LEU	95	20.664	20.608	39.757	1.00	2.18
ATOM	366	CG	LEU	95	19.934	20.373	38.438	1.00	2.18
MOTA	367	CD1		95	20.243	19.003	37.867	1.00	2.18
ATOM	368	CD2	LEU	95	18.445	20.557	38.649	1.00	2.18
						21.150	40.829	1.00	2.00
MOTA	369	C	LEU	95	22.863			1.00	2.18
ATOM	370	0	LEU	95	22.262	21.753	41.717		
MOTA	371	N	SER	96	24.168	21.305	40.606	1.00	21.89
MOTA	372	CA	SER	96	25.009	22.206	41.414	1.00	21.89
MOTA	373	CB	SER	96	26.497	21.998	41.101	1.00	46.05
ATOM	374	OG	SER	96	26.868	20.628	41.129	1.00	46.05
ATOM	375	C	SER	96	24.675	23.679	41.215	1.00	21.89
ATOM	376	Ó	SER	96	24.844	24.223	40.122	1.00	46.05
ATOM	377	N	ARG	97	24.166	24.312	42.266	1.00	23.50
ATOM	378	CA	ARG	97.	23.831	25.734	42.214	1.00	23.50
				97		26.553	42.134	1.00	38.04
ATOM	379	CB	ARG		25.128			1.00	38.04
ATOM	380	CG	ARG	97	25.891	26.663	43.424		
ATOM	381	CD	ARG	97	25.228	27.665	44.345	1.00	38.04
MOTA	382	NE	ARG	97	26.077	27.967	45.493	1.00	38.04
ATOM	383	CZ	ARG	97	25.800	28.884	46.422	1.00	38.04
ATOM	384	NH1	ARG	97	24.686	29.619	46.351	1.00	38.04
ATOM	385	NH2	ARG	97	26.643	29.058	47.439	1.00	38.04
ATOM	386	C	ARG	97	22.964	26.037	40.991	1.00	23.50
ATOM	387	ō	ARG	97	23.340	26.838	40.150	1.00	38.04
ATOM	388	N	PRO	98	21.798	25.384	40.871	1.00	46.09
ATOM	389	CD	PRO	98	21.195	24.520	41.896	1.00	35.22
			PRO	98	20.873	25.573	39.736	1.00	46.09
ATOM	390	CA						1.00	35.22
MOTA	391	CB	PRO	98	19.630	24.787	40.166		
ATOM	392	CG	PRO	98	19.723	24.759	41.683	1.00	35.22
MOTA	393	С	PRO	98	20.528	27.027	39.400	1.00	46.09
MOTA	394	0	PRO	98	20.320	27.376	38.228	1.00	35.22
MOTA	395	N	PHE	99	20.507	27.865	40.430	1.00	24.90
MOTA	396	CA	PHE	99	20.192	29.286	40.306	1.00	24.90
MOTA	397	CB	PHE	99	19.490	29.740	41.585	1.00	11.96
ATOM	398	CG	PHE	99	20.122	29.194	42.831	1.00	11.96
ATOM	399		PHE	99	21.164	29.879	43.454	1.00	11.96
ATOM	400		PHE	99	19.724	27.964	43.338	1.00	11.96
				99	21.804	29.348	44.556	1.00	11.96
MOTA	401		PHE			27.418			11.96
ATOM	402		PHE	99	20.353		44.439	1.00	
ATOM	403	CZ	PHE	99	21.401	28.108	45.053	1.00	11.96
MOTA	404	C	PHE	99	21.420	30.169	40.058	1.00	24.90
ATOM	405	0	PHE	99	21.334	31.381	40.173	1.00	11.96
MOTA	406	N	GLN	100	22.555	29.588	39.695	1.00	11.02
MOTA	407	CA	GLN	100	23.751	30.394	39.462	1.00	11.02
ATOM	408	CB	GLN	100	24.942	29.520	39.089	1.00	30.87
ATOM	409	CG	GLN	100	24.666	28.644	37.920	1.00	30.87
ATOM	410	CD	GLN	100	25.797	27.707	37.635	1.00	30.87
ATOM	411		GLM	100	26.602	27.945	36.736	1.00	30.87
AI ON		OET	GTTIA	100	20.002				



# FIG. 3H

							20 200	1 00	30.87
MOTA	412	NE2		100	25.870	26.622	38.399	1.00	
ATOM	413	C	GLN	100	23.531	31.470	38.397	1.00	11.02
MOTA	414	0	GLN	100	24.109	32.553	38.495	1.00	30.87
MOTA	415	N	ASN	101	22.746	31.144	37.363	1.00	17.49
ATOM	416	CA	ASN	101	22.414	32.077	36.288	1.00	17.49
ATOM	417	CB	ASN	101	23.525	32.176	35.220	1.00	4.38
ATOM	418	CG	ASN	101	24.074	30.827	34.774	1.00	4.38
ATOM	419	OD1	ASN	101	23.393	30.060	34.095	1.00	4.38
ATOM	420	ND2	ASN	101	25.337	30.564	35.100	1.00	4.38
MOTA	421	C	ASN	101	21.044	31.739	35.699	1.00	17.49
ATOM	422	0	ASN	101	20.607	30.602	35.759	1.00	4.38
ATOM	423	N	GLN	102	20.363	32.750	35.167	1.00	9.50
ATOM	424	CA	GLN	102	19.019	32.597	34.603	1.00	9.50
MOTA	425	CB	GLN	102	18.500	33.916	34.018	1.00	10.21
MOTA	426	CG	GLN	102	18.213	35.035	34.991	1.00	10.21
	427	CD	GLN	102	17.250	36.039	34.397	1.00	10.21
ATOM	428		GLN	102	16.111	35.689	34.091	1.00	10.21
MOTA				102	17.699	37.288	34.210	1.00	10.21
ATOM	429			102	18.886	31.546	33.531	1.00	9.50
ATOM	430	C	GLN		17.784	31.107	33.256	1.00	10.21
MOTA	431	0	GLN	102	19.978	31.228	32.844	1.00	2.00
MOTA	432	N	THR	103		30.202	31.812	1.00	2.00
MOTA	433	CA	THR	103	19.922	30.202	30.920	1.00	25.55
ATOM	434	CB	THR	103	21.194			1.00	25.55
MOTA	435	OG1	THR	103	21.433	31.565	30.460	1.00	25.55
MOTA	436	CG2	THR	103	21.022	29.327	29.693		23.33
MOTA	437	C	THR	103	19.754	28.863	32.538	1.00	25.55
ATOM	438	0	THR	103	18.848	28.088	32.232	1.00	
MOTA	439	N	HIS	104	20.574	28.656	33.570	1.00	2.12
MOTA	440	CA	HIS	104	20.525	27.455	34.412	1.00	2.12
MOTA	441	CB	HIS	104	21.704	27.415	35.382	1.00	27.31
ATOM	442	CG	HIS	104	22.953	26.854	34.794	1.00	27.31
ATOM	443	CD2	HIS	104	23.166	25.754	34.034	1.00	27.31
ATOM	444	ND1	HIS	104	24.186	27.434	34.984	1.00	27.31
MOTA	445	CE1	HIS	104	25.109	26.712	34.373	1.00	27.31
MOTA	446	NE2	HIS	104	24.513	25.687	33.788	1.00	27.31
ATOM	447	С	HIS	104	19.252	27.426	35.231	1.00	2.12
ATOM	448	0	HIS	104	18.685	26.371	35.460	1.00	27.31
ATOM	449	N	ALA	105	18.812	28.590	35.669	1.00	2.00
ATOM	450	CA	ALA	105	17.626	28.687	36.482	1.00	2.00
ATOM	451	CB	ALA	105	17.581	30.013	37.154	1.00	17.66
MOTA	452	C	ALA	105	16.348	28.433	35.710	1.00	2.00
ATOM	453	Ō	ALA	105	15.419	27.836	36.240	1.00	17.66
ATOM	454	N	LYS	106	16.307	28.827	34.444	1.00	11.55
ATOM	455	CA	LYS	106	15.109	28.606	33.635	1.00	11.55
MOTA	456	CB	LYS	106	15.102	29.507	32.392	1.00	26.36
ATOM	457	CG	LYS	106	14.999	31.015	32.716	1.00	26.36
MOTA	458	CD	LYS	106	14.630	31.862	31.518	1.00	26.36
MOTA	459	CE	LYS	106	13.149	31.713	31.135	1.00	26.36
ATOM	460	NZ	LYS	106	12.724	30.333	30.676	1.00	26.36
	461	C	LYS	106	14.982	27.132	33.251	1.00	11.55
ATOM	462	0	LYS	106	13.892	26.554	33.326	1.00	26.36
ATOM				107	16.109	26.516	32.898	1.00	16.17
ATOM	463	N	ARG		16.131	25.111	32.524	1.00	16.17
ATOM	464	CA	ARG	107	17.491	24.743	31.938	1.00	38.14
MOTA	465	CB	ARG	107	17.491	23.395	31.262	1.00	38.14
MOTA	466	CG	ARG	107	18.669	23.246	30.326	1.00	38.14
MOTA	467	CD	ARG	107	18.425	22.252	29.275	1.00	38.14
MOTA	468	NE	ARG	107	18.425	22.439	28.214	1.00	38.14
ATOM	469	CZ	ARG	107		23.593	28.034	1.00	38.14
MOTA	470	NH.	L ARG	107	16.979	23.333	20.004	2.00	

## FIG. 3I

MOTA	471	NH2	ARG	107	17.533	21.479	27.296	1.00	38.14
MOTA	472	C	ARG	107	15.790	24.179	33.697	1.00	16.17
MOTA	473	0	ARG	107	14.959	23.275	33.551	1.00	38.14
MOTA	474	N	ALA	108	16.441	24.396	34.844	1.00	17.90
MOTA	475	CA	ALA	108	16.218	23.606	36.058	1.00	17.90
ATOM	476	СВ	ALA	108	17.224	23.987	37.114	1.00	2.00
ATOM	477	С	ALA	108	14.796	23.753	36.609	1.00	17.90
ATOM	478	0	ALA	108	14.223	22.790	37.115	1.00	2.00
ATOM	479	N	TYR	109	14.219	24.944	36.502	1.00	2.00
ATOM	480	CA	TYR	109	12.875	25.158	36.987	1.00	2.00
MOTA	481	CB	TYR	109	12.548	26.642	37.069	1.00	6.75
. ATOM	482	CG	TYR	109	11.139	26.885	37.544	1.00	6.75
MOTA	483	CD1	TYR	109	10.791	26.671	38.871	1.00	6.75 6.75
MOTA	484	CE1	TYR	109	9.487	26.868	39.314	1.00	
ATOM	485	CD2	TYR	109	10.146	27.308	36.668	1.00	6.75
ATOM	486	CE2	TYR	109	8.840	27.511	37.106	1.00	6.75
MOTA	487	CZ	TYR	109	8.518	27.290	38.430	1.00	6.75
ATOM	488	OH	TYR	109	7.235	27.513	38.878	1.00	6.75
MOTA	489	C	TYR	109	11.857	24.463	36.100	1.00	2.00
MOTA	490	0	TYR	109	10.923	23.840	36.589	1.00	6.75
MOTA	491	N	ARG	110	12.027	24.630	34.793	1.00	20.21
ATOM	492	CA	ARG	110	11.162	24.042	33.771	1.00	20.21
ATOM	493	CB	ARG	110	11.536	24.628	32.414	1.00	16.32
ATOM	494	CG	ARG	110	10.586	24.328	31.279	1.00	16.32
ATOM	495	CD	ARG	110	10.990	25.137	30.058	1.00	16.32
ATOM	496	NE	ARG	110	10.184	24.829	28.884	1.00	16.32 16.32
MOTA	497	CZ	ARG	110	10.648	24.190	27.817	1.00	16.32
MOTA	498		ARG	110	11.915	23.799	27.780	1.00	
ATOM	499		ARG	110	9.846	23.940	26.788	1.00 1.00	16.32 20.21
ATOM	500	C	ARG	110	11.314	22.521	33.754	1.00	16.32
ATOM	501	0	ARG	110	10.361	21.793 22.046	33.482 34.019	1.00	2.00
ATOM	502	N	GLU	111	12.525	20.620	34.019	1.00	2.00
ATOM	503	CA	GLU	111	12.800	20.396	34.387	1.00	23.79
ATOM	504	CB	GLU	111	14.287 14.728	18.938	34.585	1.00	23.79
MOTA	505	CD	GLU	111 111	16.264	18.775	34.635	1.00	23.79
ATOM	506		GLU	111	16.753	17.651	34.352	1.00	23.79
ATOM	507 508	OE1		111	16.974	19.772	34.948	1.00	23.79
ATOM	509	C	GLU	111	11.932	20.029	35.189	1.00	2.00
ATOM ATOM	510	0	GLU	111	11.141	19.127	34.954	1.00	23.79
ATOM	511	N	LEU	112	12.045	20.599	36.384	1.00	21.88
ATOM	512	CA	LEU	112	11.288	20.171	37.559	1.00	21.88
ATOM	513	CB	LEU	112	11.518	21.150	38.701	1.00	6.65
ATOM	514	CG	LEU	112	12.563	20.834	39.746	1.00	6.65
ATOM	515		LEU	112	12.811	22.079	40.558	1.00	6.65
ATOM	516		LEU	112	12.065	19.700	40.605	1.00	6.65
ATOM	517	C	LEU	112	9.792	20.105	37.333	1.00	21.88
ATOM	518	Ö	LEU	112	9.156	19.092	37.609	1.00	6.65
ATOM	519	И	VAL	113	9.239	21.212	36.851	1.00	2.68
ATOM	520	CA	VAL	113	7.812	21.344	36.614	1.00	2.68
ATOM	521	CB	VAL	113	7.452	22.784	36.139	1.00	23.11
ATOM	522		VAL	113	5.945	22.958	36.101	1.00	23.11
ATOM	523		VAL	113	8.092	23.836	37.059	1.00	23.11
ATOM	523	C	VAL	113	7.239	20.321	35.639	1.00	2.68
ATOM	525	o	VAL	113	6.336	19.569	35.991	1.00	23.11
MOTA	526	N	LEU	114	7.800	20.251	34.437	1.00	19.44
ATOM	527	CA	LEU	114	7.321	19.327	33.413	1.00	19.44
ATOM	528	CB	LEU	114	7.894	19.701	32.054	1.00	5.29
ATOM	529	CG	LEU		7.360	21.018	31.517	1.00	5.29
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FIG. 3J

ATOM	530	CD1	LEU	114	8.103	21.355	30.254	1.00	5.29
ATOM	531	CD2	LEU	114	5.862	20.915	31.278	1.00	5.29
MOTA	532	С	LEU	114	7.606	17.869	33.714	1.00	19.44
ATOM	533	0	LEU	114	6.760	17.000	33.488	1.00	5.29
ATOM	534	N	MET	115	8.793	17.590	34.227	1.00	2.00
MOTA	535	CA	MET	115	9.128	16.227	34.565	1.00	2.00
ATOM	536	CB	MET	115	10.598	16.115	34.949	1.00	7.04
ATOM	537	CG	MET	115	11.196	14.779	34.598	1.00	7.04
ATOM	538	SD	MET	115	12.885	14.586	35.145	1.00	7.04
MOTA	539	CE	MET	115	13.731	15.695	34.061	1.00	7.04
ATOM	540	С	MET	115	8.239	15.774	35.727	1.00	2.00
MOTA	541	0	MET	115	8.217	14.597	36.067	1.00	7.04
ATOM	542	N	LYS	116	7.515	16.716	36.335	1.00	7.50
ATOM	543	CA	LYS	116	6.624	16.408	37.443	1.00	7.50
ATOM	544	CB	LYS	116	6.748	17.443	38.561	1.00	25.41
ATOM	545	CG	LYS	116	7.889	17.235	39.557	1.00	25.41
ATOM	546	CD	LYS	116	7.633	18.102	40.780	1.00	25.41
ATOM	547	CE	LYS	116	8.655	17.895	41.893	1.00	25.41
ATOM	548	NZ	LYS	116	8.311	18.681	43.125	1.00	25.41
MOTA	549	C	LYS	116	5.161	16.296	37.044	1.00	7.50
ATOM	550 551	0	LYS	116	4.409	15.572	37.692	1.00	25.41
ATOM ATOM	551 552	N CA	CYS	117 117	4.764	16.993 16.987	35.978	1.00	18.55
ATOM	552 553	CB	CYS	117	3.368 2.865	18.421	35.509 35.322	1.00 1.00	18.55 28.53
ATOM	554	SG	CYS	117	3.668	19.290	33.963	1.00	28.53
ATOM	555	C	CYS	117	3.083	16.188	34.225	1.00	18.55
ATOM	556	Ö	CYS	117	1.919	15.914	33.908	1.00	28.53
ATOM	557	N	VAL	118	4.135	15.847	33.482	1.00	13.50
ATOM	558	CA	VAL	118	4.005	15.086	32.242	1.00	13.50
ATOM	559	CB	VAL	118	5.103	15.475	31.230	1.00	25.80
ATOM	560		VAL	118	4.988	14.640	29.972	1.00	25.80
ATOM	561		VAL	118	5.014	16.942	30.906	1.00	25.80
ATOM	562	C	VAL	118	4.163	13.604	32.528	1.00	13.50
ATOM	563	0	VAL	118	5.118	13.199	33.201	1.00	25.80
ATOM	564	N	THR	119	3.244	12.784	32.021	1.00	29.88
ATOM	565	CA	THR	119	3.346	11.344	32.239	1.00	29.88
MOTA	566	CB	THR	119	2.433	10.845	33.386	1.00	46.17
ATOM	567	OG1	THR	119	2.862	9.540	33.795	1.00	46.17
ATOM	568	CG2	THR	119	0.954	10.796	32.961	1.00	46.17
ATOM	569	C	THR	119	3.153	10.534	30.966	1.00	29.88
MOTA	570	0	THR	119	2.049	10.406	30.424	1.00	46.17
MOTA	571	N	HIS	120	4.264	9.982	30.498	1.00	11.14
ATOM	572	CA	HIS	120	4.270	9.200	29.278	1.00	11.14
MOTA	573	CB		120		10.139	28.094	1.00	12.95
ATOM	574	CG	HIS	120	4.469	9.443	26.767	1.00	12.95
MOTA	575		HIS	120	5.426	9.387	25.825	1.00	12.95
MOTA	576		HIS	120	3.416	8.680	26.302	1.00	12.95
MOTA	577		HIS	120	3.737	8.183	25.118	1.00	12.95
ATOM	578	NE2		120	4.947	8.594	24.805	1.00	12.95
MOTA	579	C	HIS	120	5.432	8.227	29.351	1.00	11.14
ATOM	580 581	0	HIS	120	6.454	8.526	29.966	1.00	12.95
ATOM	581	N	LYS	121	5.271	7.071	28.717	1.00	2.00
MOTA MOTA	582 583	CA	LYS	121	6.294	6.036	28.730	1.00	2.00
ATOM	583 584	CB	LYS	121	5.700 5.028	4.697 4.721	28.281	1.00	11.42
ATOM	585	CG CD	LYS	121 121	4.423	3.362	26.918 26.545	1.00	11.42
ATOM	586	CE	LYS	121	5.478	2.269	26.451	1.00 1.00	11.42 11.42
ATOM	587	NZ	LYS	121	6.495	2.546	25.396	1.00	11.42
ATOM	588	C	LYS	121	7.550	6.349	27.928	1.00	2.00
	200	_	13		,.550	0.040	220	1.00	2.00



## FIG. 3K

ATOM	589	0	LYS	121	8.584	5.713	28.124	1.00	11.42
MOTA	590	N	asn	122	7.475	7.370	27.073	1.00	13.02
ATOM	591	CA	ASN	122	8.605	7.763	26.220	1.00	13.02
MOTA	592	CB	asn	122	8.180	7.770	24.753	1.00	2.00
MOTA	593	CG	ASN	122	7.642	6.432	24.295	1.00	2.00
MOTA	594	OD1	ASN	122	6.520	6.337	23.812	1.00	2.00
MOTA	595	ND2	ASN	122	8.438	5.385	24.470	1.00	2.00
ATOM	596	С	ASN	122	9.242	9.089	26.592	1.00	13.02
ATOM	597	0	ASN	122	10.095	9.596	25.863	1.00	2.00
MOTA	598	N	ILE	123	8.788	9.647	27.715	1.00	11.02
MOTA	599	CA	ILE	123	9.282	10.903	28.283	1.00	11.02 2.63
MOTA	600	CB	ILE	123	8.175	11.965	28.434	1.00	
ATOM	601	CG2	ILE	123	8.750	13.204	29.091	1.00	2.63 2.63
ATOM	602	CG1	ILE	123	7.588	12.333	27.074	1.00	
ATOM	603	CD1	ILE	123	8.553	13.063	26.168	1.00	2.63 11.02
MOTA	604	С	ILE	123	9.759	10.514	29.671	1.00	
MOTA	605	0	ILE	123	9.046	9.825	30.397	1.00	2.63
ATOM	606	N	ILE	124	10.932	10.998	30.070	1.00	18.75
MOTA	607	CA	ILE	124	11.501	10.629	31.368	1.00	18.75
ATOM	608	CB	ILE	124	12.940	11.205	31.577	1.00	5.83
MOTA	609	CG2	ILE	124	12.891	12.679	31.928	1.00	5.83
ATOM	610	CG1	ILE	124	13.693	10.418	32.650	1.00	5.83
MOTA	611	CD1	ILE	124	14.175	9.055	32.209	1.00	5.83
ATOM	612	C	ILE	124	10.602	10.926	32.569	1.00	18.75
ATOM	613	0	ILE	124	9.856	11.916	32.604	1.00	5.83
MOTA	614	N	SER	125	10.626	9.978	33.505	1.00	32.81
ATOM	615	CA	SER	125	9.846	10.012	34.740	1.00	32.81
ATOM	616	CB	SER	125	9.218	8.631	34.983	1.00	33.06
ATOM	617	OG	SER	125	10.203	7.594	35.025	1.00	33.06
ATOM	618	С	SER	125	10.698	10.393	35.937	1.00	32.81
ATOM	619	0	SER	125	11.807	9.881	36.126	1.00	33.06
ATOM	620	N	LEU	126	10.163	11.299	36.742	1.00	19.68
ATOM	621	CA	LEU	126	10.849	11.761	37.937	1.00	19.68
ATOM	622	CB	LEU	126	10.559	13.246	38.161	1.00	2.00
MOTA	623	CG	LEU	126	11.407	13.970	39.195	1.00	2.00
ATOM	624		LEU	126	12.855	13.566	39.085	1.00	2.00
ATOM	625	CD2	LEU	126	11.254	15.460	38.982	1.00	2.00
MOTA	626	C	LEU	126	10.387	10.919	39.127	1.00	19.68
ATOM	627	0	LEU	126	9.218	10.937	39.503	1.00	2.00
ATOM	628	N	LEU	127	11.311	10.129	39.659	1.00	23.39
ATOM	629	CA	LEU	127	11.040	9.251	40.794	1.00	23.39
MOTA	630	CB	LEU	127	11.991	8.051	40.765	1.00	2.00
ATOM	631	CG	LEU	127	11.746	6.927	39.773	1.00	2.00
ATOM	632	CD1	LEU	127	12.846	5.917	39.958	1.00	2.00
ATOM	633		LEU	127	10.390	6.305	40.018		2.00
MOTA	634	С	LEU	127	11.111	9.910	42.182	1.00	23.39
MOTA	635	O	LEU	127	10.273	9.631	43.044		2.00
ATOM	636	N	ASN	128	12.098	10.779	42.387	1.00	2.00
ATOM	637	CA	ASN	128	12.267	11.440	43.668		2.00
ATOM	638	СВ	ASN	128	12.896	10.460	44.659	1.00	16.49
MOTA	639	CG	ASN		12.913		46.077	1.00	16.49
ATOM	640		L ASN		12.031	11.729	46.494	1.00	16.49
ATOM	641		2 ASN		13.903	10.556	46.839	1.00	16.49
MOTA	642		ASN		13.128			1.00	2.00
ATOM	643		ASN		14.205			1.00	16.49
ATOM	644		VAL		12.649			1.00	19.28
MOTA	645				13.376			1.00	19.28
MOTA	646		VAL		12.480			1.00	10.22
ATOM	647		1 VAL		13.340			1.00	10.22
AIOM	0-1	CG.	سده ب			_ : : - : -			



## FIG. 3L

ATOM	648	CG2	VAL	129	11.543	15.699	42.478	1.00	10.22
ATOM	649	C	VAL	129	13.769	15.374	45.504	1.00	19.28
MOTA	650	0	VAL	129	12.944	15.238	46.401	1.00	10.22
MOTA	651	N	PHE	130	15.020	15.765	45.733	1.00	13.60
MOTA	652	CA	PHE	130	15.440	16.107	47.084	1.00	13.60
MOTA	653	CB	PHE	130	15.681	14.838	47.923	1.00	3.04
MOTA	654	CG	PHE	130	16.870	14.036	47.487	1.00	3.04
ATOM	655	CD1		130	18.136	14.317	47.987	1.00	3.04
ATOM	656	CD2	PHE	130	16.721	13.012	46.566	1.00	3.04
MOTA	657	CE1	$_{ m PHE}$	130	19.238	13.595	47.575	1.00	3.04
ATOM	658	CE2	PHE	130	17.810	12.279	46.140	1.00	3.04
MOTA	659	CZ	PHE	130	19.078	12.572	46.645	1.00	3.04
MOTA	660	С	PHE	130	16.637	17.038	47.182	1.00	13.60
ATOM	661	0	PHE	130	17.422	17.179	46.244	1.00	3.04
ATOM	662	N	THR	131	16.746	17.677	48.345	1.00	2.00
ATOM	663	CA	THR	131	17.831	18.588	48.643	1.00	2.00
ATOM	664	CB	THR	131	17.365	20.080	48.645	1.00	12.19
MOTA	665	OG1	THR	131	18.444	20.930	49.036	1.00	12.19
ATOM	666	CG2	THR	131	16.190	20.301	49.583	1.00	12.19
MOTA	667	С	THR	131	18.424	18.243	50.001	1.00	2.00
MOTA	668	0	THR	131	17.706	17.952	50.957	1.00	12.19
ATOM	669	N	PRO	132	19.753	18.182	50.072	1.00	3.54
MOTA	670	CD	PRO	132	20.704	18.219	48.952	1.00	3.20
MOTA	671	CA	PRO	132	20.447	17.875	51.315	1.00	3.54
MOTA	672	CB	PRO	132	21.815	17.428	50.827	1.00	3.20
MOTA	673	CG	PRO	132	22.045	18.285	49.661	1.00	3.20
MOTA	674	C	PRO	132	20.545	19.130	52.189	1.00	3.54
MOTA	675	0	PRO	132	21.321	19.164	53.141	1.00	3.20
ATOM	676	N	GLN	133	19.817	20.183	51.825	1.00	4.78
ATOM	677	CA	GLN	133	19.837	21.417	52.594	1.00	4.78
ATOM	678	CB	GLN	133	20.255	22.593	51.726	1.00	4.25
MOTA	679	CG	GLN	133	21.706	22.500	51.244	1.00	4.25
ATOM	680	CD	GLN	133	21.842	22.103	49.776	1.00	4.25
MOTA	681	OE1	GLN	133	22.938	21.782	49.313	1.00	4.25
MOTA	682	NE2	GLN	133	20.740	22.158	49.031	1.00	4.25
MOTA	683	C	GLN	133	18.491	21.664	53.261	1.00	4.78
MOTA	684	0	GLN	133	17.438	21.627	52.614	1.00	4.25
MOTA	685	N	LYS	134	18.543	21.913	54.570	1.00	33.73
MOTA	686	CA	LYS	134	17.347	22.134	55.373	1.00	33.73
MOTA	687	CB	LYS	134	17.641	21.862	56.857	1.00	32.87
ATOM	688	CG	LYS	134	17.725	20.379	57.225	1.00	32.87
ATOM	689	CD	LYS	134	16.352	19.667	57.154	1.00	32.87
MOTA	690	CE	LYS	134	16.477	18.156	57.418	1.00	32.87
ATOM	691	NZ	LYS	134	17.282	17.463	56.353	1.00	32.87
ATOM	692	C	LYS	134	16.658	23.482	55.220	1.00	33.73
ATOM	693	0	LYS	134	15.423	23.541	55.152	1.00	32.87
MOTA	694	N	THR	135	17.445	24.558	55.169	1.00	47.73
ATOM	695	CA	THR	135	16.883	25.905	55.046	1.00	47.73
ATOM	696	CB	THR	135	17.509	26.874	56.046	1.00	14.84
ATOM	697	OG1	THR	135	18.863	27.134	55.663	1.00	14.84
ATOM	698	CG2	THR	135	17.472	26.278	57.447	1.00	14.84
MOTA	699	C	THR	135	16.987	26.548	53.673	1.00	47.73
ATOM	700	0	THR	135	17.947	26.333	52.935	1.00	14.84
ATOM	701	N	LEU	136	16.040	27.442	53.412	1.00	2.00
MOTA	702	CA	LEU	136	15.947	28.175	52.161	1.00	2.00
ATOM	703	CB	LEU	136	14.675	29.013	52.200	1.00	7.33
ATOM	704	CG	LEU	136	14.233	29.957	51.082	1.00	7.33
ATOM	705		LEU	136	14.722	29.512	49.713	1.00	7.33
ATOM	706		LEU	136	12.702	30.046	51.146	1.00	7.33

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#### FIG. 3M

MOTA	707	C	LEU	136	17.183	29.042	51.963	1.00	2.00
MOTA	708	0	LEU	136	17.423	29.556	50.879	1.00	7.33
MOTA	709	N	GLU	137	17.952	29.217	53.034	1.00	31.36
MOTA	710	CA	GLU	137	19.174	29.997	52.971	1.00	31.36
MOTA	711	CB	GLU	137	19.468	30.699	54.311	1.00	31.26 31.26
MOTA	712	CG	GLU	137	18.689	31.988	54.571	1.00	
MOTA	713	CD	GLU	137	17.217	31.746	54.824	1.00	31.26
MOTA	714	OE1		137	16.874	31.316	55.954	1.00	31.26
MOTA	715	OE2	GLU	137	16.408	31.995	53.897	1.00	31.26
MOTA	716	С	GLU	137	20.308	29.046	52.643	1.00	31.36
MOTA	717	0	GLU	137	21.187	29.365	51.843	1.00	31.26
MOTA	718	N	GLU	138	20.296	27.885	53.290	1.00	18.21
MOTA	719	CA	GLU	138	21.323	26.876	53.059	1.00	18.21
MOTA	720	CB	GLU	138	21.201	25.760	54.080	1.00	15.04
MOTA	721	CG	GLU	138	21.529	26.161	55.492	1.00	15.04
MOTA	722	CD	$\mathtt{GLU}$	138	21.167	25.065	56.475	1.00	15.04
ATOM	723	OE1		138	20.996	25.388	57.667	1.00	15.04
MOTA	724	OE2	GLU	138	21.046	23.881	56.049	1.00	15.04
MOTA	725	C	GLU	138	21.215	26.264	51.668	1.00	18.21
MOTA	726	0	GLU	138	22.184	25.693	51.167	1.00	15.04
MOTA	727	N	PHE	139	20.026	26.381	51.078	1.00	16.05
ATOM	728	CA	PHE	139	19.706	25.843	49.766	1.00	16.05
ATOM	729	CB	PHE	139	18.343	26.391	49.310	1.00	31.29
MOTA	730	CG	PHE	139	17.847	25.800	48.009	1.00	31.29
MOTA	731	CD1	PHE	139	17.879	24.422	47.802	1.00	31.29
MOTA	732	CD2	PHE	139	17.385	26.619	46.982	1.00	31.29
MOTA	733	CE1	PHE	139	17.467	23.867	46.588	1.00	31.29
MOTA	734	CE2	PHE	139	16.967	26.082	45.760	1.00	31.29
ATOM	735	CZ	PHE	139	17.008	24.703	45.561	1.00	31.29
ATOM	736	C	PHE	139	20.786	26.105	48.709	1.00	16.05
MOTA	737	0	PHE	139	21.061	27.256	48.350	1.00	31.29
MOTA	738	N	GLN	140	21.414	25.036	48.231	1.00	2.00
MOTA	739	CA	GLN	140	22.466	25.157	47.241	1.00	2.00
MOTA	740	CB	GLN	140	23.820	24.911	47.898	1.00	31.26
MOTA	741	CG	GLN	140	24.966	25.054	46.954	1.00	31.26
MOTA	742	CD	GLN	140	26.264	25.266	47.672	1.00	31.26
ATOM	743	OE1	GLN	140	26.386	26.183	48.482	1.00	31.26
ATOM	744	NE2	GLN	140	27.253	24.416	47.386	1.00	31.26
ATOM	745	C	GLN	140	22.287	24.258	46.020	1.00	2.00
MOTA	746	0	GLN	140	22.262	24.757	44.894	1.00	31.26
MOTA	747	N	ASP	141	22.185	22.946	46.230	1.00	10.22
MOTA	748	CA	ASP	141	22.022	22.008	45.125	1.00	10.22
MOTA	749	CB	ASP	141	23.152	20.980	45.123	1.00	13.10
MOTA	750	CG	ASP	141	24.524	21.613	45.146	1.00	13.10
MOTA	751		ASP	141	24.732	22.666	44.515	1.00	13.10
MOTA	752	OD2	ASP	141	25.418	21.070	45.815	1.00	13.10
MOTA	753	C	ASP	141	20.684	21.285	45.179	1.00	10.22
ATOM	754	0	ASP	141	19.991	21.323	46.199	1.00	13.10
MOTA	755	N	VAL	142	20.308	20.675	44.055	1.00	6.00
MOTA	756	CA	VAL	142	19.070	19.901	43.923	1.00	6.00
MOTA	757	CB	VAL	142	18.043	20.631	43.043	1.00	2.00
MOTA	758	CG1	. VAL	142	16.789	19.783	42.866	1.00	2.00
MOTA	759		VAL	142	17.696	21.962	43.672	1.00	2.00
MOTA	760	C	VAL	142	19.425	18.552	43.296	1.00	6.00
MOTA	761	0	VAL	142	20.270	18.486	42.412	1.00	2.00
ATOM	762	N	TYR	143	18.814	17.475	43.789	1.00	3.45
MOTA	763	CA	TYR	143	19.089	16.130	43.289	1.00	3.45
MOTA	764	CB	TYR	143	19.607	15.227	44.405	1.00	2.80
MOTA	765	CG	TYR	143	20.990	15.557	44.878	1.00	2.80



## FIG. 3N

MOTA	766	CD1	TYR	143	21.217	16.619	45.739	1.00	2.80
MOTA	767	CE1	TYR	143	22.493	16.932	46.171	1.00	2.80
MOTA	768	CD2	TYR	143	22.078	14.813	44.459	1.00	2.80
ATOM	769	CE2	TYR	143	23.362	15.120	44.882	1.00	2.80
ATOM	770	CZ	TYR	143	23.567	16.184	45.736	1.00	2.80
ATOM	771	OH	TYR	143	24.849	16.513	46.129	1.00	2.80
ATOM	772	C	TYR	143	17.848	15.509	42.691	1.00	3.45
ATOM	773	ō	TYR	143	16.846	15.331	43.376	1.00	2.80
ATOM	774	N	LEU	144	17.915	15.193	41.401	1.00	20.45
ATOM	775	CA	LEU	144	16.789	14.578	40.694	1.00	20.45
ATOM	776	CB	LEU	144	16.635	15.173	39.284	1.00	5.98
ATOM	777	CG	LEU	144	16.571	16.690	39.101	1.00	5.98
ATOM	778		LEU	144	16.787	17.000	37.651	1.00	5.98
ATOM	779		LEU	144	15.246	17.268	39.574	1.00	5.98
	780	C	LEU	144	17.032	13.078	40.575	1.00	20.45
ATOM			LEU	144	18.152	12.639	40.286	1.00	5.98
ATOM	781	0			15.991	12.294	40.835	1.00	6.79
ATOM	782	N	VAL	145	16.102	10.841	40.738	1.00	6.79
ATOM	783	CA	VAL	145			42.113	1.00	2.00
ATOM	784	CB	VAL	145	15.889	10.161		1.00	2.00
MOTA	785		VAL	145	15.824	8.671	41.951		2.00
MOTA	786		VAL	145	17.015	10.525	43.056	1.00	
MOTA	787	C	VAL	145	15.124	10.269	39.720	1.00	6.79
ATOM	788	0	VAL	145	13.911	10.416	39.853	1.00	2.00
MOTA	789	N	MET	146	15.652	9.658	38.671	1.00	19.74
MOTA	790	CA	MET	146	14.792	9.060	37.657	1.00	19.74
MOTA	791	CB	MET	146	14.943	9.773	36.319	1.00	10.11
MOTA	792	CG	MET	146	14.723	11.253	36.405	1.00	10.11
ATOM	793	SD	MET	146	16.115	12.116	35.673	1.00	10.11
MOTA	794	CE	MET	146	17.511	11.529	36.681	1.00	10.11
MOTA	795	С	MET	146	15.189	7.607	37.533	1.00	19.74
MOTA	796	0	MET	146	15.972	7.101	38.329	1.00	10.11
MOTA	797	N	GLU	147	14.654	6.934	36.526	1.00	2.00
ATOM	798	CA	GLU	147	14.961	5.531	36.312	1.00	2.00
MOTA	799	CB	GLU	147	13.923	4.906	35.419	1.00	35.81
ATOM	800	CG	GLU	147	12.537	5.132	35.881	1.00	35.81
ATOM	801	CD	GLU	147	11.530	4.438	35.011	1.00	35.81
MOTA	802	OE1	GLU	147	11.914	3.602	34.152	1.00	35.81
ATOM	803	OE2	GLU	147	10.338	4.732	35.201	1.00	35.81
MOTA	804	С	GLU	147	16.299	5.352	35.658	1.00	2.00
ATOM	805	0	GLU	147	16.846	6.274	35.067	1.00	35.81
ATOM	806	N	LEU	148	16.801	4.135	35.720	1.00	2.00
ATOM	807	CA	LEU	148	18.060	3.847	35.097	1.00	2.00
ATOM	808	CB	LEU	148	18.962	3.091	36.052	1.00	2.00
ATOM	809	CG	LEU	148	20.399	3.148	35.568	1.00	2.00
ATOM	810		LEU	148	20.940	4.544	35.769	1.00	2.00
ATOM	811		LEU	148	21.228	2.139	36.303	1.00	2.00
ATOM	812	C	LEU	148	17.872	3.066	33.792	1.00	2.00
ATOM	813	ō	LEU	148	17.317	1.963	33.759	1.00	2.00
ATOM	814	N	MET	149	18.305	3.698	32.711	1.00	12.82
ATOM	815	CA	MET	149	18.251	3.120	31.387	1.00	12.82
ATOM	816	CB	MET	149	18.097	4.207	30.335	1.00	5.88
		CG	MET	149	16.934	5.107	30.610	1.00	5.88
ATOM	817			149	15.478	4.137	30.863	1.00	5.88
ATOM	818	SD	MET	149	14.727	4.137	29.246	1.00	5.88
ATOM	819	CE	MET						
ATOM	820	C	MET	149	19.585	2.434	31.218	1.00	12.82
ATOM	821	0	MET	149	20.474	2.572	32.065	1.00	5.88
ATOM	822	N	ASP	150	19.741	1.723	30.106	1.00	5.65
ATOM	823	CA	ASP	150	20.971	0.996	29.856	1.00	5.65
MOTA	824	CB	ASP	150	20.631	-0.351	29.256	1.00	4.35
				•					



FIG. 30

ATOM	825	CG	ASP	150	19.680	-1.122	30.110	1.00	4.35
ATOM	826	OD1	ASP	150	19.847	-1.096	31.342	1.00	4.35
MOTA	827	OD2	ASP	150	18.746	-1.729	29.575	1.00	4.35
MOTA	828	С	ASP	150	22.042	1.695	29.067	1.00	5.65
ATOM	829	0	ASP	150	23.211	1.326	29.168	1.00	4.35
ATOM	830	N	ALA	151	21.654	2.701	28.292	1.00	2.00
MOTA	831	CA	ALA	151	22.595	3.461	27.474	1.00	2.00
ATOM	832	CB	ALA	151	23.152	2.568	26.364	1.00	2.00
ATOM	833	C	ALA	151	21.920	4.673	26.855	1.00	2.00
ATOM	834	Ō	ALA	151	20.741	4.914	27.071	1.00	2.00
ATOM	835	N	ASN	152	22.692	5.445	26.100	1.00	23.78
ATOM	836	CA	ASN	152	22.163	6.613	25.401	1.00	23.78
ATOM	837	CB	ASN	152	23.103	7.832	25.525	1.00	36.42
ATOM	838	CG	ASN	152	24.481	7.596	24.918	1.00	36.42
ATOM	839		ASN	152	24.621	6.905	23.910	1.00	36.42
ATOM	840		ASN	152	25.499	8.190	25.524	1.00	36.42
ATOM	841	C	ASN	152	21.906	6.262	23.921	1.00	23.78
ATOM	842	Ö	ASN	152	22.289	5.186	23.446	1.00	36.42
ATOM	843	N	LEU	153	21.282	7.182	23.193	1.00	11.01
MOTA	844	CA	LEU	153	20.984	6.954	21.783	1.00	11.01
ATOM	845	CB	LEU	153	19.923	7.924	21.297	1.00	2.00
ATOM	846	CG	LEU	153	18.761	7.314	20.526	1.00	2.00
	847		LEU	153	18.173	8.369	19.610	1.00	2.00
ATOM ATOM	848		LEU	153	19.220	6.129	19.727	1.00	2.00
		CDZ	LEU	153	22.208	7.056	20.872	1.00	11.01
ATOM ATOM	849		LEU	153	22.203	6.504	19.783	1.00	2.00
	850	0		154	23.260	7.728	21.330	1.00	12.15
MOTA	851	N	CYS			7.720	20.532	1.00	12.15
MOTA	852	CA	CYS	154	24.462 25.243	9.131	20.964	1.00	53.10
MOTA	853	CB	CYS	154		8.917	22.444	1.00	53.10
ATOM	854	SG	CYS	154	26.248	6.645	20.589	1.00	12.15
MOTA	855	C	CYS	154	25.337 26.325	6.538	19.862	1.00	53.10
ATOM	856	0	CYS	154	24.971	5.713	21.466	1.00	2.99
ATOM	857	N	GLN	155	25.683	4.455	21.604	1.00	2.99
ATOM	858	CA	GLN	155		3.913	23.016	1.00	16.88
ATOM	859	CB	GLN	155	25.533	4.461	24.027	1.00	16.88
ATOM	860	CG	GLN	155	26.518	3.868	25.414	1.00	16.88
ATOM	861	CD	GLN	155	26.286 25.385	4.292	26.139	1.00	16.88
ATOM	862	OE1		155	27.088	2.872	25.777	1.00	16.88
ATOM	863	NE2		155		3.488	20.635	1.00	2.99
ATOM	864	C	GLN	155	25.033		20.055	1.00	16.88
ATOM	865	0	GLN	155	25.693	2.638 3.637	20.033	1.00	12.86
ATOM	866	N	VAL	156	23.721 22.916	2.816	19.579	1.00	12.86
ATOM	867	CA	VAL	156			19.839	1.00	2.00
ATOM	868		VAL	156	21.399 20.539	3.055	18.731	1.00	2.00
MOTA	869		VAL	156		2.462	21.181	1.00	2.00
ATOM	870		VAL	156	20.999	2.484		1.00	12.86
MOTA	871	C	VAL	156	23.249	3.203	18.123	1.00	2.00
ATOM	872	0	VAL	156	22.997	2.460	17.175		10.11
ATOM	873	N	ILE	157	23.834	4.380	17.970	1.00	10.11
ATOM	874	CA	ILE	157	24.213	4.893	16.683	1.00	
ATOM	875	CB	ILE	157	24.291	6.432	16.755	1.00	8.01
ATOM	876		ILE	157	25.350	6.997	15.812	1.00	8.01
ATOM	877		ILE	157	22.904	6.994	16.453	1.00	8.01
ATOM	878		ILE	157	22.730	8.386	16.893	1.00	8.01
ATOM	879	C	ILE	157	25.520	4.263	16.235	1.00	10.11
ATOM	880	0	ILE	157	25.806	4.196	15.039		8.01
MOTA	881	N	GLN		26.286	3.743	17.184	1.00	2.00
ATOM	882	CA	GLN	158	27.551	3.106	16.853	1.00	2.00
MOTA	883	CB	GLN	158	28.533	3.251	18.005	1.00	52.31



## FIG. 3P

MOTA	884	CG	GLN	158	29.150	4.613	18.169	1.00	52.31
MOTA	885	CD	GLN	158	30.188	4.613	19.276	1.00	52.31
MOTA	886	OE1	GLN	158	31.112	3.786	19.272	1.00	52.31
MOTA	887	NE2	GLN	158	30.034	5.521	20.246	1.00	52.31
MOTA	888	C	GLN	158	27.396	1.628	16.507	1.00	2.00
MOTA	889	0	GLN	158	28.381	0.886	16.483	1.00	52.31
MOTA	890	N	MET	159	26.159	1.190	16.298	1.00	2.84
MOTA	891	CA	MET	159	25.890	-0.197	15.956	1.00	2.84
MOTA	892	CB	MET	159	25.516	-0.978	17.203	1.00	12.08 12.08
ATOM	893	CG	MET	159	24.130	-0.673	17.736	1.00	
ATOM	894	SD	MET	159	24.057	-0.915	19.488	1.00	12.08
MOTA	895	CE	MET	159	22.779	-2.121	19.575	1.00 1.00	12.08 2.84
ATOM	896	C	MET	159	24.760	-0.265	14.937	1.00	12.08
MOTA	897	0	MET	159	23.749	0.428	15.059	1.00	2.00
ATOM	898	N	GLU	160	24.921	-1.118 -1.254	13.937 12.899	1.00	2.00
ATOM	899	CA	GLU	160	23.916	-1.933	11.663	1.00	23.86
ATOM	900	CB	GLU	160	24.518 25.306	-3.189	11.973	1.00	23.86
MOTA	901	CG	GLU	160	25.643	-3.189	10.730	1.00	23.86
ATOM	902	CD	GLU	160 160	26.618	-3.588	10.730	1.00	23.86
ATOM	903	OE1	GLU	160	24.938	-4.987	10.471	1.00	23.86
ATOM	904	OE2 C	GLU	160	22.711	-2.032	13.396	1.00	2.00
MOTA MOTA	905 906	0	GLU	160	22.847	-3.137	13.899	1.00	23.86
ATOM	907	N	LEU	161	21.530	-1.443	13.254	1.00	5.79
ATOM	908	CA	LEU	161 ·	20.292	-2.074	13.713	1.00	5.79
ATOM	909	CB	LEU	161	19.462	-1.071	14.510	1.00	13.20
ATOM	910	CG	LEU	161	20.034	-0.330	15.703	1.00	13.20
ATOM	911		LEU	161	19.066	0.772	16.064	1.00	13.20
ATOM	912		LEU	161	20.249	-1.293	16.857	1.00	13.20
ATOM	913	C	LEU	161	19.392	-2.600	12.598	1.00	5.79
ATOM	914	ō	LEU	161	19.435	-2.113	11.466	1.00	13.20
ATOM	915	N	ASP	162	18.559	-3.582	12.933	1.00	7.84
ATOM	916	CA	ASP	162	17.606	-4.121	11.977	1.00	7.84
ATOM	917	CB	ASP	162	17.054	-5.477	12.449	1.00	9.47
MOTA	918	CG	ASP	162	16.717	-5.502	13.942	1.00	9.47
ATOM	919	OD1	ASP	162	17.654	-5.665	14.759	1.00	9.47
MOTA	920	OD2	ASP	162	15.517	-5.390	14.292	1.00	9.47
MOTA	921	C	ASP	162	16.478	-3.083	11.857	1.00	7.84
MOTA	922	0	ASP	162	16.405	-2.161	12.667	1.00	9.47
MOTA	923	N	HIS	163	15.629	-3.202	10.836	1.00	22.67
MOTA	924	CA	HIS	163	14.513	-2.265	10.642	1.00	22.67
MOTA	925	CB	HIS	163	13.807	-2.537	9.322	1.00	13.35
MOTA	926	CG	HIS	163	14.651	-2.254	8.127	1.00	13.35
MOTA	927	CD2		163	14.985	-3.032	7.069	1.00	13.35 13.35
ATOM	928		HIS	163	15.260	-1.038 -1.074	7.916 6.783	1.00 1.00	13.35
MOTA	929		HIS	163	15.932	-2.275	6.249	1.00	13.35
ATOM	930		HIS	163	15.783	-2.255	11.764	1.00	22.67
ATOM	931	C	HIS	163	13.471 12.824	-1.238	11.784	1.00	13.35
ATOM	932	0	HIS	163	13.316	-3.379	12.465	1.00	21.78
ATOM	933	N CA	GLU	164 164	12.345	-3.498	13.564	1.00	21.78
ATOM	934	CB	GLU	164	12.221	-4.960	14.005	1.00	11.17
ATOM	935 936	CG	GLU	164 164	11.194	-5.786	13.232	1.00	11.17
ATOM	936	CD	GLU	164	11.437	-5.819	11.734	1.00	11.17
ATOM ATOM	938		GLU.	164	10.452	-5.639	10.989	1.00	11.17
ATOM	939	OE2		164	12.595	-6.035	11.294	1.00	11.17
MOTA	939	C	GLU	164	12.721	-2.631	14.760	1.00	21.78
ATOM	941	Ö	GTA	164	11.955	-1.782	15.206	1.00	11.17
ATOM	942	N	ARG		13.926	-2.845	15.257	1.00	2.00
ALON	742	~*	211.0	100					



# FIG. 3Q

ATOM	943	CA	ARG	165	14.439	-2.094	16.373	1.00	2.00
MOTA	944	CB	ARG	165	15.839	-2.582	16.714	1.00	23.45
MOTA	945	CG	ARG	165	15.866	-3.907	17.467	1.00	23.45
MOTA	946	CD	ARG	165	17.304	-4.246	17.862	1.00	23.45
MOTA	947	NE	ARG	165	17.397	-5.350	18.807	1.00	23.45
MOTA	948	CZ	ARG	165	17.137	-6.622	18.516	1.00	23.45
MOTA	949	NH1	ARG	165	16.759	-6.984	17.297	1.00	23.45
MOTA	950	NH2	ARG	165	17.260	-7.542	19.454	1.00	23.45
ATOM	951	С	ARG	165	14.480	-0.624	16.017	1.00	2.00
MOTA	952	0	ARG	165	13.924	0.201	16.728	1.00	23.45
ATOM	953	N	MET	166	15.120	-0.310	14.897	1.00	2.00
MOTA	954	CA.	MET	166	15.252	1.061	14.407	1.00	2.00
ATOM	955	CB	MET	166	15.915	1.046	13.031	1.00	28.00
MOTA	956	CG	MET	166	16.291	2.401	12.473	1.00	28.00
MOTA	957	SD	MET	166	16.936	2.244	10.786	1.00	28.00
MOTA	958	CE	MET	166	18.697	1.770	11.111	1.00	28.00
MOTA	959	C	MET	166	13.897	1.781	14.340	1.00	2.00
MOTA	960	0	MET	166	13.766	2.913	14.809	1.00	28.00
ATOM	961	N	SER	167	12.887	1.106	13.790	1.00	12.38
ATOM	962	CA	SER	167	11.537	1.655	13.666	1.00	12.38
ATOM	963	CB	SER	167	10.715	0.830	12.683	1.00	11.87
MOTA	964	OG	SER	167	10.651	-0.522	13.100	1.00	11.87
MOTA	965	C	SER	167	10.788	1.746	14.996	1.00	12.38 11.87
MOTA	966	0	SER	167	9.874	2.568	15.129	1.00	2.00
ATOM	967	N	TYR	168	11.130	0.891	15.962	1.00	2.00
MOTA	968	CA	TYR	168	10.481	0.938	17.266	1.00	4.15
MOTA	969	CB	TYR	168	10.763	-0.322	18.088	1.00 1.00	4.15
MOTA	970	CG	TYR	168	9.916	-0.389	19.328 19.263	1.00	4.15
MOTA	971		TYR	168	8.543	-0.155	20.406	1.00	4.15
MOTA	972	CE1		168	7.750	-0.148	20.406	1.00	4.15
ATOM	973	CD2		168	10.479 9.692	-0.629 -0.625	21.733	1.00	4.15
MOTA	974	CE2		168	8.325	-0.381	21.733	1.00	4.15
ATOM	975	CZ	TYR	168	7.544	-0.357	22.780	1.00	4.15
MOTA	976	OH	TYR	168 168	11.007	2.162	18.004	1.00	2.00
ATOM	977	C	TYR	168	10.250	2.102	18.626	1.00	4.15
ATOM	978	N O	TYR LEU	169	12.317	2.352	17.919	1.00	4.07
ATOM	979 980	CA.	LEU	169	12.970	3.482	18.526	1.00	4.07
MOTA		CA	LEU	169	14.482	3.400	18.292	1.00	4.89
ATOM	981 982	CG	LEU	169	15.256	2.291	19.009	1.00	4.89
MOTA MOTA	983		LEU	169	16.746	2.558	18.881	1.00	4.89
ATOM	984		LEU	169	14.864	2.262	20.477	1.00	4.89
ATOM	985	C	LEU	169	12.379	4.759	17.915	1.00	4.07
ATOM	986	ō	LEU	169	11.830	5.595	18.634	1.00	4.89
ATOM	987	N	LEU	170	12.373	4.843	16.587	1.00	2.00
ATOM	988	CA	LEU	170	11.834	6.008	15.888	1.00	2.00
ATOM	989	CB	LEU	170	12.027	5.869	14.382	1.00	5.04
MOTA	990	CG	LEU	170	13.257	6.551	13.776	1.00	5.04
ATOM	991		LEU	170	13.065	8.058	13.715	1.00	5.04
ATOM	992		FEU	170	14.485	6.194	14.585	1.00	5.04
ATOM	993	C	LEU	170	10.359	6.268	16.198	1.00	2.00
ATOM	994	ō	LEU	170	9.949	7.421	16.334	1.00	5.04
ATOM	995	N	TYR	171	9.573	5.205	16.351	1.00	22.09
ATOM	996	CA	TYR	171	8.151	5.340	16.669	1.00	22.09
ATOM	997	CB	TYR	171	7.452	3.981	16.530	1.00	9.28
ATOM	998	CG	TYR	171	6.110	3.846	17.219	1.00	9.28
ATOM	999		LTYR	171	4.939	4.328	16.634	1.00	9.28
MOTA	1000		LTYR	171	3.696	4.181	17.278	1.00	9.28
MOTA	1001		YYR	171	6.009	3.209	18.460	1.00	9.28



## FIG. 3R

MOTA	1002	CE2	TYR	171	4.777	3.063	19.110	1.00	9.28
MOTA	1003	CZ	TYR	171	3.628	3.551	18.515	1.00	9.28
MOTA	1004	OH	TYR	171	2.412	3.411	19.152	1.00	9.28
ATOM	1005	С	TYR	171	7.982	5.915	18.081	1.00	22.09
MOTA	1006	0	TYR	171	7.074	6.717	18.337	1.00	9.28
ATOM	1007	N	GLN	172	8.879	5.529	18.986	1.00	2.00
ATOM	1008	CA	GLN	172	8.830	6.020	20.346	1.00	2.00
ATOM	1009	CB	GLN	172	9.698	5.164	21.251	1.00	13.55
ATOM	1010	CG	GLN	172	9.162	3.775	21.454	1.00	13.55
ATOM	1011	CD	GLN	172	10.033	2.976	22.376	1.00	13.55
ATOM	1012	OE1	GLN	172	9.758	2.867	23.576	1.00	13.55
MOTA	1013	NE2	GLN	172	11.109	2.424	21.834	1.00	13.55
ATOM	1014	C	GLN	172	9.244	7.479	20.411	1.00	2.00
MOTA	1015	0	GLN	172	8.676	8.254	21.183	1.00	13.55
MOTA	1016	N	MET	173	10.202	7.871	19.582	1.00	4.17
ATOM	1017	CA	MET	173	10.642	9.255	19.569	1.00	4.17
ATOM	1018	CB	MET	173	11.800	9.452	18.612	1.00	2.80
MOTA	1019	CG	MET	173	13.130	9.233	19.241	1.00	2.80
MOTA	1020	SD	MET	173	14.412	9.163	18.023	1.00	2.80
MOTA	1021	ÇE	MET	173	14.864	7.494	18.142	1.00	2.80
MOTA	1022	С	MET	173	9.487	10.128	19.144	1.00	4.17
MOTA	1023	0	MET	173	9.307	11.218	19.672	1.00	2.80
ATOM	1024	N	LEU	174	8.696	9.637	18.195	1.00	6.58
ATOM	1025	CA	LEU	174	7.544	10.387	17.711	1.00	6.58
ATOM	1026	CB	LEU	174	7.069	9.857	16.346	1.00	2.00
MOTA	1027	CG	LEU	174	8.065	9.936	15.177	1.00	2.00
MOTA	1028	CD1	LEU	174	7.532	9.144	13.998	1.00	2.00
ATOM	1029	CD2	LEU	174	8.336	11.393	14.784	1.00	2.00
MOTA	1030	C	LEU	174	6.395	10.426	18.730	1.00	6.58
MOTA	1031	0	LEU	174	5.728	11.456	18.881	1.00	2.00
MOTA	1032	N	CYS	175	6.181	9.332	19.455	1.00	4.87
ATOM	1033	CA	CYS	175	5.118	9.310	20.450	1.00	4.87
ATOM	1034	CB	CYS	175	4.966	7.909	21.033	1.00	2.00
MOTA	1035	SG	CYS	175	4.104	6.748	19.992	1.00	2.00
ATOM	1036	С	CYS	175	5.411	10.321	21.564	1.00	4.87
MOTA	1037	0	CYS	175	4.552	11.119	21.943	1.00	2.00
MOTA	1038	N	GLY	176	6.659	10.315	22.027	1.00	2.00
ATOM	1039	CA	GLY	176	7.093	11.207	23.076	1.00	2.00
ATOM	1040	С	GLY	176	7.004	12.652	22.651	1.00	2.00
MOTA	1041	0	GLY	176	6.575	13.497	23.425	1.00	28.56
MOTA	1042	N	ILE	177	7.373	12.935	21.410	1.00	14.73
ATOM	1043	CA	ILE	177	7.336	14.293	20.882	1.00	14.73
MOTA	1044	CB	ILE	177	8.222	14.419	19.643	1.00	2.00
ATOM	1045	CG2	ILE	177	8.085	15.773	19.020	1.00	2.00
MOTA	1046	CG1	ILE	177	9.676	14.229	20.040	1.00	2.00
MOTA	1047	CD1	ILE	177	10.542	13.878	18.869	1.00	2.00
MOTA	1048	C	ILE	177	5.911	14.721	20.562	1.00	14.73
ATOM	1049	0	ILE	177	5.592	15.908	20.584	1.00	2.00
MOTA	1050	N	LYS	178	5.034	13.758	20.311	1.00	2.00
MOTA	1051	CA	LYS	178	3.659	14.107	20.027	1.00	2.00
MOTA	1052	CB	LYS	178	2.906	12.991	19.310	1.00	12.67
MOTA	1053	CG	LYS	178	1.564	13.501	18.827	1.00	12.67
ATOM	1054	CD	LYS	178	0.546	12.434	18.593	1.00	12.67
ATOM	1055	CE	LYS	178	-0.785	13.112	18.357	1.00	12.67
ATOM	1056	NZ	LYS	178	-1.854	12.145	18.059	1.00	12.67
MOTA	1057	C	LYS	178	2.944	14.456	21.311	1.00	2.00
MOTA	1058	0	LYS	178	2.028	15.263	21.304	1.00	12.67
MOTA	1059	N	HIS	179	3.343	13.833	22.411	1.00	2.00
MOTA	1060	CA	HIS	179	2.729	14.110	23.708	1.00	2.00

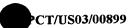


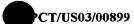
FIG. 35

									5.57
ATOM	1061	CB	HIS	179	3.168	13.074	24.740	1.00	
ATOM	1062	CG	HIS	179	2.349	13.086	25.993	1.00	5.57
ATOM	1063	CD2	HIS	179	2.678	13.396	27.267	1.00	5.57
ATOM	1064	ND1	HIS	179	1.014	12.743	26.011	1.00	5.57
ATOM	1065	CE1		179	0.554	12.849	27.243	1.00	5.57
MOTA	1066	NE2	HIS	179	1.545	13.240	28.026	1.00	5.57
ATOM	1067	С	HIS	179	3.178	15.497	24.147	1.00	2.00
ATOM	1068	ō	HIS	179	2.405	16.278	24.697	1.00	5.57
ATOM	1069	N	LEU	180	4.437	15.799	23.871	1.00	2.00
	1070	CA	LEU	180	5.002	17.086	24.193	1.00	2.00
ATOM		CB	LEU	180	6.438	17.165	23.674	1.00	5.28
ATOM	1071			180	7.537	17.357	24.713	1.00	5.28
MOTA	1072	CG	LEU	180	7.412	16.299	25.773	1.00	5.28
MOTA	1073				8.892	17.305	24.063	1.00	5.28
MOTA	1074		LEU	180		18.154	23.509	1.00	2.00
MOTA	1075	С	LEU	180	4.151		24.143	1.00	5.28
ATOM	1076	0	LEU	180	3.695	19.095	22.225	1.00	2.00
ATOM	1077	N	HIS	181	3.883	17.958		1.00	2.00
MOTA	1078	CA	HIS	181	3.092	18.901	21.458	1.00	9.13
ATOM	1079	CB	HIS	181	3.194	18.578	19.976		9.13
MOTA	1080	CG	HIS	181	4.602	18.599	19.449	1.00	
MOTA	1081	CD2	HIS	181	5.768	18.916	20.034	1.00	9.13
MOTA	1082	ND1	HIS	181	4.895	18.279	18.144	1.00	9.13
ATOM	1083	CE1	HIS	181	6.196	18.407	17.950	1.00	9.13
ATOM	1084	NE2	HIS	181	6.752	18.792	19.077	1.00	9.13
ATOM	1085	C	HIS	181	1.626	18.934	21.877	1.00	2.00
ATOM	1086	0	HIS	181	0.941	19.937	21.662	1.00	9.13
ATOM	1087	N	SER	182	1.151	17.857	22.501	1.00	38.18
ATOM	1088	CA	SER	182	-0.235	17.762	22.970	1.00	38.18
ATOM	1089	CB	SER	182	-0.630	16.305	23.248	1.00	31.08
ATOM	1090	OG	SER	182	0.004	15.791	24.408	1.00	31.08
	1090	C	SER	182	-0.413	18.612	24.227	1.00	38.18
ATOM	1091	o	SER	182	-1.520	19.065	24.534	1.00	31.08
MOTA		N	ALA	183	0.690	18.799	24.951	1.00	14.47
ATOM	1093			183	0.711	19.609	26.159	1.00	14.47
ATOM	1094	CA	ALA ALA	183	1.670	19.014	27.160	1.00	4.36
ATOM	1095	CB			1.104	21.057	25.830	1.00	14.47
MOTA	1096	C	ALA	183	1.148	21.037	26.712	1.00	4.36
MOTA	1097	0	ALA	183		21.316	24.554	1.00	2.00
MOTA	1098	N	GLY	184	1.382		24.113	1.00	2.00
MOTA	1099	CA	GLY	184	1.766	22.644	24.113	1.00	2.00
MOTA	1100	C	GLY	184	3.262	22.893		1.00	17.40
MOTA	1101	0	GLY	184	3.691	24.046	24.081	1.00	2.00
MOTA	1102	N	ILE	185	4.047	21.826	24.370		2.00
ATOM	1103	CA	ILE	185	5.511	21.894	24.464	1.00	
MOTA	1104	CB	ILE	185	6.041	20.899	25.514	1.00	4.90
MOTA	1105	CG2	2 ILE	185	7.532	21.128	25.750	1.00	4.90
MOTA	1106	CG:	1 ILE	185	5.244	21.006	26.808	1.00	4.90
MOTA	1107	CD:	1 ILE	185	5.464	19.851	27.766	1.00	4.90
ATOM	1108	С	ILE	185	6.205	21.541	23.153	1.00	2.00
ATOM	1109	0	ILE	185	5.973	20.468	22.613	1.00	4.90
ATOM	1110	N	ILE	186	7.077	22.423	22.666	1.00	7.82
ATOM	1111	CA		186	7.823	22.185	21.428	1.00	7.82
MOTA	1112			186	7.435	23.175	20.302	1.00	17.50
MOTA	1113		2 ILE	186	8.323	22.972		1.00	17.50
ATOM	1113		1 ILE	186	5.983			1.00	17.50
	1115		1 ILE	186	5.434	_			17.50
MOTA					9.326				7.82
ATOM	1116		ILĖ	186	9.962				17.50
MOTA	1117		ILE	186	9.872				22.00
MOTA	1118		HIS	187	11.277				22.00
MOTA	1119	CA	HIS	187	44.411	20.,02			



## FIG. 3T

					11 575	19.297	21.774	1.00	3.84
MOTA	1120	CB	HIS	187	11.575	18.623	22.682	1.00	3.84
ATOM	1121	CG	HIS	187	12.554			1.00	3.84
MOTA	1122	CD2		187	12.384	17.652	23.602	1.00	3.84
MOTA	1123	ND1		187	13.895	18.941	22.699		
ATOM	1124	CE1		187	14.509	18.191	23.594	1.00	3.84
MOTA	1125	NE2	HIS	187	13.614	17.400	24.157	1.00	3.84
MOTA	1126	С	HIS	187	12.310	21.680	21.518	1.00	22.00
ATOM	1127	0	HIS	187	12.891	22.526	22.197	1.00	3.84
MOTA	1128	N	ARG	188	12.508	21.499	20.216	1.00	6.22
ATOM	1129	CA	ARG	188	13.463	22.242	19.401	1.00	6.22
ATOM	1130	CB	ARG	188	13.201	23.739	19.445	1.00	27.37
ATOM	1131	CG	ARG	188	11.932	24.159	18.755	1.00	27.37
ATOM	1132	CD	ARG	188	11.856	25.658	18.715	1.00	27.37
MOTA	1133	NE	ARG	188	11.646	26.237	20.043	1.00	27.37
ATOM	1134	CZ	ARG	188	12.366	27.234	20.560	1.00	27.37
ATOM	1135		ARG	188	13.368	27.775	19.875	1.00	27.37
	1136		ARG	188	12.038	27.749	21.742	1.00	27.37
ATOM		C	ARG	188	14.944	21.950	19.652	1.00	6.22
ATOM	1137				15.799	22.651	19.123	1.00	27.37
MOTA	1138	0	ARG	188	15.250	20.919	20.445	1.00	12.44
MOTA	1139	N	ASP	189		20.543	20.705	1.00	12.44
MOTA	1140	CA	ASP	189	16.646		21.859	1.00	15.30
MOTA	1141	CB	ASP	189	17.240	21.367	21.833	1.00	15.30
MOTA	1142	CG	ASP	189	18.767	21.294			15.30
ATOM	1143		ASP	189	19.413	21.349	20.835	1.00	15.30
MOTA	1144	OD2	ASP	189	19.320	21.164	23.017	1.00	
ATOM	1145	С	ASP	189	16.879	19.035	20.933	1.00	12.44
MOTA	1146	0	ASP	189	17.730	18.635	21.731	1.00	15.30
MOTA	1147	N	LEU	190	16.139	18.202	20.208	1.00	2.00
MOTA	1148	CA	LEU	190	16.293	16.757	20.327	1.00	2.00
MOTA	1149	CB	LEU	190	15.263	16.035	19.467	1.00	11.08
ATOM	1150	CG	LEU	190	13.848	16.009	20.029	1.00	11.08
MOTA	1151	CD1	LEU	190	12.872	16.076	18.889	1.00	11.08
MOTA	1152	CD2	LEU	190	13.618	14.777	20.900	1.00	11.08
ATOM	1153	С	LEU	190	17.680	16.353	19.860	1.00	2.00
ATOM	1154	Ō	LEU	190	18.072	16.672	18.755	1.00	11.08
ATOM	1155	N	LYS	191	18.432	15.680	20.715	1.00	2.00
ATOM	1156	CA	LYS	191	19.764	15.222	20.357	1.00	2.00
ATOM	1157	СВ	LYS	191	20.829	16.200	20.852	1.00	15.76
MOTA	1158	CG	LYS	191	20.620	16.731	22.261	1.00	15.76
ATOM	1159	CD	LYS	191	21.700	17.727	22.660	1.00	15.76
ATOM	1160	CE	LYS	191	21.478	19.088	22.025	1.00	15.76
ATOM	1161		LYS	191	22.411	20.123	22.562	1.00	15.76
	1162	. RZ	LYS	191	19.932	13.829	20.941	1.00	2.00
ATOM			LYS	191	19.342	13.518	21.954	1.00	15.76
MOTA	1163	0		192	20.669	12.944	20.259	1.00	8.42
MOTA	1164	N	PRO		21.359	13.131	18.973	1.00	6.93
MOTA	1165	CD	PRO	192	20.872	11.579	20.756	1.00	8.42
MOTA	1166	CA	PRO	192		11.032	19.809	1.00	6.93
MOTA	1167	CB	PRO	192	21.939			1.00	6.93
MOTA	1168	CG	PRO	192	21.594	11.704	18.522		8.42
MOTA	1169	C	PRO	192	21.318	11.529	22.205	1.00	
MOTA	1170	0	PRO	192	20.848	10.697	22.985	1.00	6.93
MOTA	1171	N	SER	193	22.190	12.464	22.576	1.00	15.86
MOTA	1172	CA	SER	193	22.699	12.527	23.935	1.00	15.86
ATOM	1173	CB	SER	193	23.830		24.063	1.00	24.60
MOTA	1174	OG	SER	193	23.439		23.709	1.00	24.60
ATOM	1175	C	SER	193	21.582	12.804		1.00	15.86
ATOM	1176	0	SER	193	21.705	12.459	26.101	1.00	24.60
MOTA	1177	N	ASN	194	20.475	13.372	24.453	1.00	5.51
MOTA	1178	CA		194	19.327	13.685	25.306	1.00	5.51
					•				



### FIG. 3U

ATOM	1179	CB	ASN	194	18.844	15.115	25.057	1.00	7.93
MOTA	1180	CG	ASN	194	19.824	16.151	25.558	1.00	7.93
ATOM	1181	OD1	ASN	194	20.810	15.821	26.222	1.00	7.93
ATOM	1182		ASN	194	19.567	17.406	25.251	1.00	7.93
MOTA	1183	С	ASN	194	18.173	12.701	25.156	1.00	5.51
MOTA	1184	0	ASN	194	17.006	13.050	25.369	1.00	7.93
MOTA	1185	N	ILE	195	18.509	11.487	24.738	1.00	2.00
ATOM	1186	CA	ILE	195	17.549	10.414	24.570	1.00	2.00
ATOM	1187	CB	ILE	195	17.168	10.196	23.094	1.00	11.94
MOTA	1188	CG2	ILE	195	16.066	9.167	23.015	1.00	11.94
ATOM	1189	CG1	ILE	195	16.701	11.496	22.446	1.00	11.94
.ATOM	1190	CD1	ILE	195	16.189	11.344	21.041	1.00	11.94
MOTA	1191	С	ILE	195	18.260	9.174	25.074	1.00	2.00
ATOM	1192	0	ILE	195	19.418	8.931	24.738	1.00	11.94
ATOM	1193	N	VAL	196	17.584	8.402	25.909	1.00	2.00
ATOM	1194	CA	VAL	196	18.175	7.192	26.463	1.00	2.00
MOTA	1195	CB	VAL	196	18.364	7.288	28.004	1.00	2.00
ATOM	1196	CG1	VAL	196	19.559	8.175	28.334	1.00	2.00
ATOM	1197	CG2	VAL	196	17.104	7.831	28.680	1.00	2.00
ATOM	1198	С	VAL	196	17.379	5.948	26.100	1.00	2.00
ATOM	1199	0	VAL	196	16.164	6.010	25.887	1.00	2.00
MOTA	1200	N	VAL	197	18.083	4.816	26.018	1.00	25.26
ATOM	1201	CA	VAL	197	17.466	3.529	25.669	1.00	25.26
ATOM	1202	CB	VAL	197	17.871	3.056	24.250	1.00	3.01
ATOM	1203	CG1	VAL	197	17.301	3.987	23.196	1.00	3.01
MOTA	1204	CG2	VAL	197	19.386	2.944	24.131	1.00	3.01
ATOM	1205	С	VAL	197	17.711	2.382	26.652	1.00	25.26
MOTA	1206	0	VAL	197	18.615	2.422	27.492	1.00	3.01
MOTA	1207	N	LYS	198	16.841	1.382	26.563	1.00	8.42
MOTA	1208	CA	LYS	198	16.924	0.191	27.393	1.00	8.42
ATOM	1209	CB	LYS	198	15.583	-0.091	28.070	1.00	30.51
MOTA	1210	CG	LYS	198	15.690	-0.379	29.574	1.00	30.51
MOTA	1211	CD	LYS	198	14.314	-0.471	30.219	1.00	30.51
MOTA	1212	CE	LYS	198	13.538	0.837	30.039	1.00	30.51
ATOM	1213	NZ	LYS	198	12.062	0.708	30.271	1.00	30.51
MOTA	1214	C	LYS	198	17.305	-0.950	26.462	1.00	8.42
MOTA	1215	0	LYS	198	17.233	-0.812	25.238	1.00	30.51
MOTA	1216	N	SER	199	17.688	-2.082	27.041	1.00	12.70 12.70
ATOM	1217	CA	SER	199	18.096	-3.247	26.260	1.00	2.13
ATOM	1218	CB	SER	199	18.808	-4.261	27.154 27.628	1.00 1.00	2.13
MOTA	1219 1220	C OG	SER	199 199	20.040 16.929	-3.730 -3.898	25.518	1.00	12.70
ATOM	1221	0	SER	199	17.110	-4.445	24.440	1.00	2.13
MOTA		N	SER	200	15.730	-3.795	26.091		2.00
MOTA	1222 1223	CA	ASP ASP	200	14.526	-4.362	25.484	1.00	2.00
ATOM ATOM	1224	CB	ASP	200	13.440	-4.653	26.536	1.00	13.93
ATOM	1225	CG	ASP	200	12.980	-3.410	27.300	1.00	13.93
ATOM	1225		ASP	200	12.159	-3.554	28.228	1.00	13.93
MOTA	1227		ASP	200	13.434	-2.294	26.997	1.00	13.93
ATOM	1228	C	ASP	200	13.968	-3.444	24.424	1.00	2.00
ATOM	1229	ŏ	ASP	200	12.801	-3.553	24.054		13.93
ATOM	1230	N	CYS	201	14.794	-2.475	24.027	1.00	34.23
ATOM	1231	CA	CYS	201	14.459	-1.494	23.002	1.00	34.23
ATOM	1232	CB	CYS	201	14.047	-2.221	21.712	1.00	23.39
ATOM	1233	SG	CYS	201	14.806	-1.561	20.216	1.00	23.39
ATOM	1234	C	CYS	201	13.427	-0.417	23.384	1.00	34.23
ATOM	1235	ō	CYS	201	12.812	0.196	22.521	1.00	23.39
ATOM	1236	N	THR	202	13.205	-0.203	24.671	1.00	5.40
MOTA	1237	CA	THR	202	12.267	0.841	25.065	1.00	5.40



## FIG. 3V

ATOM	1238	СВ	THR	202	11.569	0.533	26.393	1.00	3.53
ATOM	1239	OG1	THR	202	12.519	0.015	27.325	1.00	3.53
MOTA	1240	CG2	THR	202	10.450	-0.470	26.181	1.00	3.53
MOTA	1241	C	THR	202	13.026	2.154	25.122	1.00	5.40
ATOM	1242	0	THR	202	14.192	2.184	25.519	1.00	3.53
MOTA	1243	N	LEU	203	12.375	3.231	24.696	1.00	6.11
MOTA	1244	CA	LEU	203	13.022	4.537	24.641	1.00	6.11
MOTA	1245	CB	LEU	203	13.267	4.898	23.160	1.00	2.00
ATOM	1246	CG	LEU	203	13.898	6.228	22.739	1.00	2.00 2.00
MOTA	1247		LEU	203	14.745	6.067	21.485	1.00	2.00
ATOM	1248	CD2	LEU	203	12.805	7.260	22.537	1.00	6.11
MOTA	1249	C	LEU	203	12.318	5.678	25.384	1.00 1.00	2.00
ATOM	1250	0	PEA	203	11.093	5.743	25.440	1.00	2.00
ATOM	1251	N	LYS	204	13.126	6.580	25.943	1.00	2.00
MOTA	1252	CA	LYS	204	12.640	7.749	26.679 28.189	1.00	15.81
ATOM	1253	CB	LYS	204	12.649	7.484	28.713	1.00	15.81
ATOM	1254	CG	LYS	204	11.461	6.691	30.176	1.00	15.81
MOTA	1255	CD	LYS	204	11.669	6.344	30.178	1.00	15.81
MOTA	1256	CE	LYS	204	10.467 9.735	5.612 6.418	31.772	1.00	15.81
ATOM	1257	NZ	LYS	204		9.003	26.386	1.00	2.00
ATOM	1258	C	LYS	204	13.473 14.664	8.929	26.300	1.00	15.81
ATOM	1259	0	LYS	204 205	12.822	10.155	26.457	1.00	2.00
MOTA	1260	N	ILE	205	13.467	11.437	26.222	1.00	2.00
ATOM	1261	CA CB	ILE	205	12.566	12.327	25.335	1.00	4.27
ATOM	1262 1263	CG2	ILE	205	13.193	13.713	25.165	1.00	4.27
ATOM ATOM	1264	CG1	ILE	205	12.375	11.623	23.978	1.00	4.27
ATOM	1265	CD1	ILE	205	11.334	12.228	23.067	1.00	4.27
ATOM	1266	C	ILE	205	13.746	12.082	27.578	1.00	2.00
ATOM	1267	Ö	ILE	205	12.885	12.099	28.454	1.00	4.27
MOTA	1268	N	LEU	206	14.966	12.590	27.744	1.00	9.54
MOTA	1269	CA	LEU	206	15.401	13.212	28.995	1.00	9.54
ATOM	1270	CB	LEU	206	16.916	13.070	29.149	1.00	2.00
ATOM	1271	CG	LEU	206	17.509	11.665	29.133	1.00	2.00
ATOM	1272		LEU	206	19.016	11.740	29.282	1.00	2.00
ATOM	1273		LEU	206	16.895	10.831	30.240	1.00	2.00
ATOM	1274	С	LEU	206	14.975	14.669	29.236	1.00	9.54
ATOM	1275	0	LEU	206	14.370	14.961	30.265	1.00	2.00
ATOM	1276	N	ASP	207	15.279	15.568	28.298	1.00	2.00
MOTA	1277	CA	ASP	207	14.922	16.984	28.433	1.00	2.00
ATOM	1278	CB	ASP	207	16.142	17.877	28.130	1.00	21.09
MOTA	1279	CG	ASP	207	16.622	17.795	26.672	1.00	21.09
MOTA	1280	OD1	ASP	207	16.316	16.816	25.946	1.00	21.09
MOTA	1281	OD2	ASP	207	17.334	18.734	26.248	1.00	21.09
MOTA	1282	C	ASP	207	13.694	17.442	27.628	1.00	2.00
MOTA	1283	0	ASP	207	13.144	16.682	26.834	1.00	21.09
MOTA	1284	N	PHE	208	13.258	18.680	27.872	1.00	10.73
ATOM	1285	CA	PHE	208	12.107	19.280	27.180	1.00	10.73
MOTA	1286	CB	PHE	208	11.056	19.774	28.182	1.00	2.16
ATOM	1287	CG	PHE	208	10.493	18.678	29.054	1.00	2.16
ATOM	1288		PHE	208	11.197	18.236	30.183	1.00	2.16
MOTA	1289		PHE	208	9.297	18.052	28.720	1.00	2.16
MOTA	1290		PHE	208	10.727	17.173	30.968	1.00	2.16
ATOM	1291		PHE	208	8.809	16.986	29.493	1.00	2.16
ATOM	1292	CZ	PHE		9.528	16.539	30.622	1.00	2.16
MOTA	1293	C	PHE		12.592	20.403	26.268 25.688	1.00	10.73 2.16
ATOM	1294	0	PHE		11.814	21.161 20.484	25.000	1.00 1.00	5.67
ATOM	1295	N	GLY		13.915	20.484	25.325	1.00	5.67
ATOM	1296	CA	GLY	209	14.591	Z1.#JJ	23.323	1.00	5.07



### FIG. 3W

						00 015	05 544	1.00	5.67
MOTA	1297	С	GLY	209	14.420	22.917	25.544	1.00	33.44
MOTA	1298	0	GLY	209	14.431	23.427	26.673 24.413	1.00	21.09
MOTA	1299	N	LEU	210	14.299	23.604		1.00	21.09
MOTA	1300	CA	LEU	210	14.155	25.052	24.363	1.00	15.39
MOTA	1301	CB	LEU	210	14.411	25.531	22.928		15.39
ATOM	1302	CG	LEU	210	15.869	25.761	22.500	1.00	15.39
ATOM	1303	_	LEU	210	16.791	24.688	23.048	1.00	15.39
MOTA	1304	CD2	LEU	210	15.967	25.854	20.987	1.00	
ATOM	1305	C	LEU	210	12.806	25.553	24.868	1.00	21.09
MOTA	1306	0	LEU	210	11.781	24.872	24.740	1.00	15.39
MOTA	1307	N	ALA	211	12.825	26.740	25.466	1.00	12.93
MOTA	1308	CA	ALA	211	11.616	27.358	25.993	1.00	12.93
MOTA	1309	CB	ALA	211	11.970	28.365	27.092	1.00	26.16
MOTA	1310	С	ALA	211	10.851	28.049	24.873	1.00	12.93
MOTA	1311	0	ALA	211	11.504	28.842	24.167	1.00	26.16
ATOM	1312	CB	THR	217	20.244	32.345	26.028	1.00	51.78
MOTA	1313	OG1	THR	217	20.882	31.058	26.017	1.00	51.78
ATOM	1314	CG2	THR	217	20.335	32.984	24.649	1.00	51.78
ATOM	1315	C	THR	217	22.426	33.123	27.062	1.00	44.85
ATOM	1316	0	THR	217	23.008	32.685	26.058	1.00	51.78
MOTA	1317	N	THR	217	20.488	34.675	26.939	1.00	44.85
MOTA	1318	CA	THR	217	20.902	33.255	27.103	1.00	44.85
ATOM	1319	N	PHE	218	23.063	33.473	28.176	1.00	53.03
MOTA	1320	CA	PHE	218	24.512	33.400	28.273	1.00	53.03
MOTA	1321	СВ	PHE	218	25.091	34.820	28.360	1.00	30.03
ATOM	1322	CG	PHE	218	26.582	34.867	28.555	1.00	30.03
ATOM	1323	CD1	PHE	218	27.446	34.687	27.474	1.00	30.03
ATOM	1324		PHE	218	27.121	35.110	29.820	1.00	30.03
MOTA	1325		PHE	218	28.833	34.748	27.644	1.00	30.03
ATOM	1326		PHE	218	28.509	35.174	30.014	1.00	30.03
MOTA	1327	CZ	PHE	218	29.374	34.992	28.919	1.00	30.03
ATOM	1328	C	PHE	218	24.960	32.523	29.453	1.00	53.03
ATOM	1329	ō	PHE	218	24.265	32.409	30.478	1.00	30.03
ATOM	1330	N	MET	219	26.104	31.871	29.261	1.00	33.01
ATOM	1331	CA	MET	219	26.713	30.992	30.251	1.00	33.01
ATOM	1332	CB	MET	219	26.383	29.529	29.945	1.00	57.60
ATOM	1333	CG	MET	219	25.102	28.960	30.517	1.00	57.60
ATOM	1334	SD	MET	219	25.090	27.161	30.128	1.00	57.60
ATOM	1335	CE	MET	219	24.715	27.219	28.251	1.00	57.60
ATOM	1336	C	MET	219	28.215	31.132	30.085	1.00	33.01
ATOM	1337	Ō	MET	219	28.694	31.476	29.001	1.00	57.60
ATOM	1338	N	MET	220	28.962	30.879	31.154	1.00	36.45
MOTA	1339	CA	MET	220	30.408	30.920	31.035	1.00	36.45
ATOM	1340	CB	MET	220	31.052	31.852	32.063	1.00	15.11
ATOM	1341	CG	MET	220	31.584	33.117	31.410	1.00	15.11
ATOM	1342	SD	MET	220	32.595	34.145	32.466	1.00	15.11
ATOM	1343	CE	MET	220	31.381	35.216	33.043	1.00	15.11
ATOM	1344	C	MET	220	30.983	29.497	31.070	1.00	36.45
ATOM	1345	ō	MET	220	32.078	29.255	31.590	1.00	15.11
ATOM	1346	N	THR	221	30.234	28.568	30.473	1.00	39.69
ATOM	1347			221	30.647	27.170	30.381	1.00	39.69
ATOM	1348	СВ		221	29.474	26.227	29.943	1.00	47.10
ATOM	1349		1 THR	221	28.223		30.453	1.00	47.10
ATOM	1350		2 THR	221	29.705			1.00	47.10
ATOM	1351		THR	221	31.756			1.00	39.69
ATOM	1352		THR	221	31.746			1.00	47.10
ATOM	1353			224	30.615			1.00	24.68
ATOM	1354		1 VAL	224	30.847				24.68
ATOM	1355		2 VAL	224	29.898		21.524	1.00	24.68
<b></b>									



## FIG. 3X

ATOM	1356	С	VAL	224	28.536	22.979	23.715	1.00	32.19
ATOM	1357	0	VAL	224	28.480	21.788	24.050	1.00	24.68
ATOM	1358	N	VAL	224	30.614	23.160	25.007	1.00	32.19
ATOM	1359	CA	VAL	224	29.818	23.776	23.904	1.00	32.19
ATOM	1360	N	VAL	225	27.504	23.661	23.220	1.00	31.51
ATOM	1361	CA	VAL	225	26.195	23.055	22.963	1.00	31.51
ATOM	1362	СВ	VAL	225	25.057	24.106	23.005	1.00	14.81
ATOM	1363	CG1	VAL	225	23.715	23.408	23.114	1.00	14.81
ATOM	1364		VAL	225	25.258	25.091	24.153	1.00	14.81
ATOM	1365	С	VAL	225	26.178	22.405	21.578	1.00	31.51
MOTA	1366	0	VAL	225	26.782	22.923	20.630	1.00	14.81
MOTA	1367	N	THR	226	25.475	21.279	21.466	1.00	28.04
MOTA	1368	CA	THR	226	25.375	20.564	20.198	1.00	28.04
ATOM	1369	CB	THR	226	25.213	19.042	20.412	1.00	35.95
MOTA	1370	OG1	THR	226	26.259	18.568	21.278	1.00	35.95
ATOM	1371	CG2	THR	226	25.305	18.308	19.069	1.00	35.95
MOTA	1372	C	THR	226	24.206	21.128	19.390	1.00	28.04
MOTA	1373	0	THR	226	23.057	21.100	19.831	1.00	35.95
MOTA	1374	N	ARG	227	24.511	21.597	18.184	1.00	20.49 20.49
MOTA	1375	CA	ARG	227	23.518	22.220	17.320	1.00	27.34
MOTA	1376	CB	ARG	227	24.025	23.611	16.944	1.00	27.34
MOTA	1377	CG	ARG	227	25.440	23.563	16.354	1.00 1.00	27.34
MOTA	1378	CD	ARG	227	26.164	24.869	16.543	1.00	27.34
MOTA	1379	NE	ARG	227	25.948	25.423	17.877	1.00	27.34
ATOM	1380	CZ	ARG	227	25.822	26.721	18.134	1.00	27.34
MOTA	1381		ARG	227	25.902	27.605	17.149 19.370	1.00	27.34
MOTA	1382		ARG	227	25.567	27.140	16.041	1.00	20.49
MOTA	1383	C	ARG	227	23.236	21.450	15.293	1.00	27.34
ATOM	1384	0	ARG	227	22.315	21.793 20.410	15.803	1.00	2.02
MOTA	1385	N	TYR	228	24.020	19.634	14.584	1.00	2.02
ATOM	1386	CA	TYR	228	23.890 24.819	18.421	14.624	1.00	15.88
ATOM	1387	CB	TYR	228 228	26.211	18.676	15.146	1.00	15.88
MOTA	1388	CG	TYR	228	26.807	19.926	15.055	1.00	15.88
ATOM	1389	CE	L TYR L TYR	228	28.102	20.141	15.518	1.00	15.88
MOTA	1390		2 TYR	228	26.945	17.651	15.713	1.00	15.88
ATOM	1391 1392	CE		228	28.233	17.854	16.171	1.00	15.88
MOTA	1392	CZ	TYR	228	28.808	19.095	16.075	1.00	15.88
MOTA MOTA	1394	OH	TYR	228	30.087	19.273	16.550	1.00	15.88
MOTA	1395	C	TYR	228	22.482	19.151	14.242	1.00	2.02
MOTA	1396	o	TYR	228	22.194	18.887	13.081	1.00	15.88
ATOM	1397	N	TYR	229	21.597	19.060	15.229	1.00	16.06
ATOM	1398	CA	TYR	229	20.248	18.540	14.976	1.00	16.06
ATOM	1399	CB		229	19.909	17.421	15.992	1.00	7.45
ATOM	1400	CG		229	21.065	16.473	16.273	1.00	7.45
MOTA	1401		1 TYR	229	22.113	16.850	17.116	1.00	7.45
ATOM	1402		1 TYR	229	23.219	16.033	17.305		7.45
MOTA	1403			229	21.155	15.231	15.641		7.45
ATOM	1404			229	22.266	14.406			7.45
MOTA	1405			229	23.292	14.822	16.663		7.45
MOTA	1406	ОН		229	24.428	14.074			7.45
ATOM	1407		TYR	229	19.159				16.06
ATOM	1408		TYR	229	17.972				7.45
MOTA	1409	N	ARG	230	19.559				14.21
ATOM	1410	CA		230	18.604				14.21
ATOM	1411	CB	ARG	230	19.234				40.21
MOTA	1412	CG	ARG	230	19.643				40.21
MOTA	1413	CD	ARG	230	19.970				40.21
MOTA	1414	. NE	ARG	230	20.596	24.378	18.650	1.00	40.21



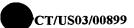
## FIG. 3Y

									1 00	40.21
MOTA	1415	CZ	ARG	230		.9.948	24.518	19.802	1.00	40.21
ATOM	1416		ARG	230		.8.635	24.720	19.805	1.00	40.21
MOTA	1417	NH2	ARG	230		0.624	24.522	20.950	1.00	14.21
MOTA	1418	C	ARG	230		.7.996	22.210	13.311	1.00	40.21
MOTA	1419	0	ARG	230		.8.669	22.095	12.283	1.00	2.00
MOTA	1420	N	ALA	231	-	L6.715	22.570	13.317	1.00	2.00
MOTA	1421	CA	ALA	231		L5.966	22.843	12.097	1.00	3.97
MOTA	1422	CB	ALA	231		L4.489	22.874	12.386	1.00	2.00
MOTA	1423	C	ALA	231		L6.423	24.164	11.494	1.00	3.97
MOTA	1424	0	ALA	231		L7.041	24.978	12.170	1.00	19.85
ATOM	1425	N	PRO	232		16.145	24.391	10.202 9.272	1.00	34.15
MOTA	1426	CD	PRO	232		15.491	23.457	-	1.00	19.85
MOTA	1427	CA	PRO	232		16.529	25.618	9.494	1.00	34.15
MOTA	1428	CB	PRO	232		16.128	25.306	8.041	1.00	34.15
MOTA	1429	CG	PRO	232		16.156	23.797	7.967	1.00	19.85
MOTA	1430	С	PRO	232		15.756	26.809	10.018	1.00	34.15
MOTA	1431	0	PRO	232		16.247	27.936	10.034	1.00	5.93
MOTA	1432	N	GLU	233		14.532	26.539	10.453	1.00	5.93
MOTA	1433	CA	GLU	233		13.657	27.567	10.984	1.00	20.38
MOTA	1434	CB	GLU	233		12.210	27.056	11.092	1.00	20.38
MOTA	1435	CG	GLU	233		12.010	25.814	11.959 11.190	1.00	20.38
MOTA	1436	CD	GLU	233		11.421	24.626	10.554	1.00	20.38
MOTA	1437		GLU	233		12.204	23.889	11.234	1.00	20.38
MOTA	1438	OE2		233		10.181	24.432	12.333	1.00	5.93
MOTA	1439	C	GLU	233		14.164	28.053		1.00	20.38
MOTA	1440	0	GLU	233		13.616	29.000	12.909	1.00	2.00
ATOM	1441	N	VAL	234		15.222	27.404	12.820	1.00	2.00
MOTA	1442	CA	VAL	234		15.855	27.745	14.079 15.002	1.00	7.29
ATOM	1443	CB	VAL	234		15.972	26.501	16.071	1.00	7.29
MOTA	1444		VAL	234		17.045	26.718	15.671	1.00	7.29
MOTA	1445		VAL	234		14.620	26.203 28.275	13.769	1.00	2.00
MOTA	1446	C	VAL	234		17.253	29.254	14.353	1.00	7.29
MOTA	1447	0	VAL	234		17.700	27.632	12.833	1.00	32.07
MOTA	1448	N	ILE	235		17.936	28.046	12.433	1.00	32.07
MOTA	1449	CA	ILE	235		19.272	27.013	11.476	1.00	7.32
MOTA	1450	CB	ILE	235		19.878	27.013	10.939	1.00	7.32
MOTA	1451	CG2		235		21.224	25.692		1.00	7.32
MOTA	1452	CG1		235		20.041	24.554		1.00	7.32
MOTA	1453	CD1		235		20.523 19.236	29.422		1.00	32.07
MOTA	1454	C	ILE	235					1.00	7.32
MOTA	1455	0	ILE	235		20.216	29.759		1.00	29.90
MOTA	1456	N	LEU	236 236		18.088 17.893	31.043		1.00	29.90
MOTA	1457	CA	LEU			17.501	30.818		1.00	2.52
MOTA	1458	CB	LEU	236 236		18.477			1.00	2.52
MOTA	1459	CG				17.772			1.00	2.52
ATOM	1460		L LEU	236		19.779			1.00	2.52
MOTA	1461		2 LEU	236 236		16.810			1.00	29.90
MOTA	1462	C	LEU			16.445			1.00	2.52
MOTA	1463	0		236 237		16.267				27.32
MOTA	1464	N	GLY	237		15.236				27.32
MOTA	1465	CA	GLY GLY			14.135				27.32
MOTA	1466	C	GLY	237 237		14.138		_		32.38
ATOM	1467	0		237		13.193				36.62
MOTA	1468	N	MET	238		12.087				36.62
ATOM	1469			238		12.134				19.68
ATOM	1470			238		11.861				19.68
MOTA	1471			238		12.644	_			19.68
ATOM	1472			238		14.336				19.68
MOTA	1473	CE	LIBI	230				<del>-</del>		



## FIG. 3Z

ATOM	1474	C	MET	238	10.718	32.091	11.662	1.00	36.62
MOTA	1475	0	MET	238	9.679	32.428	11.076	1.00	19.68
ATOM	1476	N	GLY	239	10.718	31.487	12.844	1.00	3.52
ATOM	1477	CA	GLY	239	9.470	31.105	13.472	1.00	3.52
ATOM	1478	C	GLY	239	9.390	29.604	13.327	1.00	3.52
ATOM	1479	ō	GLY	239	10.337	28.988	12.832	1.00	6.91
ATOM	1480	N	TYR	240	8.294	28.998	13.773	1.00	2.00
	1481	CA	TYR	240	8.168	27.546	13.686	1.00	2.00
MOTA		CB	TYR	240	9.241	26.864	14.570	1.00	15.34
ATOM	1482				9.198	27.170	16.070	1.00	15.34
MOTA	1483	CG	TYR	240	8.368	26.452	16.932	1.00	15.34
MOTA	1484		TYR	240			18.303	1.00	15.34
MOTA	1485	CE1	TYR	240	8.326	26.731	16.626	1.00	15.34
MOTA	1486		TYR	240	9.992	28.178		1.00	15.34
MOTA	1487	CE2	TYR	240	9.954	28.466	17.997		15.34
MOTA	1488	CZ	TYR	240	9.117	27.740	18.825	1.00	
MOTA	1489	oh	TYR	240	9.049	28.041	20.164	1.00	15.34
MOTA	1490	C	TYR	240	6.802	27.005	14.070	1.00	2.00
MOTA	1491	0	TYR	240	5.915	27.751	14.481	1.00	15.34
ATOM	1492	N	LYS	241	6.626	25.704	13.888	1.00	2.00
ATOM	1493	CA	LYS	241	5.406	25.036	14.298	1.00	2.00
ATOM	1494	СВ	LYS	241	4.376	24.928	13.166	1.00	9.47
ATOM	1495	CG	LYS	241	4.863	24.349	11.851	1.00	9.47
	1496	CD	LYS	241	3.667	24.134	10.930	1.00	9.47
MOTA		CE	LYS	241	4.050	23.720	9.511	1.00	9.47
ATOM	1497			241	2.830	23.442	8.669	1.00	9.47
MOTA	1498	NZ	LYS		5.789	23.682	14.900	1.00	2.00
ATOM	1499	C	LYS	241			15.184	1.00	9.47
MOTA	1500	0	LYS	241	6.960	23.436		1.00	3.20
MOTA	1501	N	GLU	242	4.811	22.818	15.128		3.20
MOTA	1502	CA	GLU	242	5.065	21.503	15.720	1.00	
MOTA	1503	CB	GLU	242	3.767	20.703	15.885	1.00	26.25
ATOM	1504	CG	${f GLU}$	242	2.465	21.471	15.649	1.00	26.25
ATOM	1505	CD	GLU	242	2.189	22.526	16.708	1.00	26.25
MOTA	1506	OE1	GLU	242	1.730	22.153	17.820	1.00	26.25
MOTA	1507	OE2	GLU	242	· 2.414	23.727	16.410	1.00	26.25
ATOM	1508	C	GLU	242	6.054	20.642	14.946	1.00	3.20
ATOM	1509	Ö	GLU	242	6.743	19.818	15.539	1.00	26.25
MOTA	1510	N	ASN	243	6.106	20.812	13.629	1.00	11.35
ATOM	1511	CA	ASN	243	7.002	20.013	12.799	1.00	11.35
	1512	CB	ASN	243	6.471	19.940	11.356	1.00	19.67
ATOM			ASN	243	6.636	21.251	10.578	1.00	19.67
ATOM	1513	CG			7.122	22.261	11.098	1.00	19.67
ATOM	1514		ASN	243	6.253	21.219	9.312	1.00	19.67
MOTA	1515		2 ASN	243			12.805	1.00	11.35
MOTA	1516	C	ASN	243	8.482	20.409	11.989	1.00	19.67
ATOM	1517	0	ASN	243	9.248	19.919			6.71
MOTA	1518	N	VAL	244	8.890	21.293	13.707	1.00	
MOTA	1519	CA	VAL	244	10.291	21.688	13.785	1.00	6.71
MOTA	1520	CB	VAL	244	10.478	23.032	14.569	1.00	2.00
MOTA	1521	CG:	L VAL	244	9.830	22.954	15.941	1.00	2.00
ATOM	1522	CG:	LAV S	244	11.958	23.406	14.676	1.00	2.00
ATOM	1523	C	VAL	244	11.133	20.570	14.411	1.00	6.71
ATOM	1524	ō	VAL	244	12.359	20.532	14.265	1.00	2.00
ATOM	1525	N	ASP	245	10.470	19.650	15.103	1.00	6.59
ATOM	1526	CA		245	11.154	18.527	15.738	1.00	6.59
ATOM	1527	CB	ASP	245	10.385	18.096	16.988	1.00	3.97
	1527			245	10.553	19.059	18.151	1.00	3.97
ATOM		CG		245	11.703	19.434	18.438	1.00	3.97
MOTA	1529		1 ASP		9.542	19.415	18.780	1.00	3.97
ATOM	1530		2 ASP	245		17.344	14.773	1.00	6.59
ATOM	1531	C	ASP	245	11.327				3.97
MOTA	1532	0	ASP	245	12.221	16.510	14.960	1.00	3.7/



# FIG. 3AA

MOTA	1533	N	ILE	246	10.485	17.286	13.740	1.00	9.45
ATOM	1534	CA	ILE	246	10.551	16.235	12.724	1.00	9.45
ATOM	1535	CB	ILE	246	9.405	16.375	11.676	1.00	2.00
ATOM	1536	CG2	ILE	246	9.767	15.693	10.375	1.00	2.00
MOTA	1537	CG1	ILE	246	8.093	15.809	12.238	1.00	2.00
MOTA	1538	CD1	ILE	246	8.085	14.298	12.471	1.00	2.00
MOTA	1539	C	ILE	246	11.913	16.295	12.028	1.00	9.45
MOTA	1540	0	ILE	246	12.474	15.271	11.649	1.00	2.00
ATOM	1541	N	TRP	247	12.461	17.500	11.917	1.00	2.00
MOTA	1542	CA	TRP	247	13.753	17.696	11.297	1.00	2.00
MOTA	1543	CB	TRP	247	14.049	19.183	11.127	1.00	2.00
MOTA	1544	CG	TRP	247	15.459	19.469	10.711	1.00	2.00
ATOM	1545	CD2	TRP	247	15.952	19.627	9.377	1.00	2.00
MOTA	1546	CE2	TRP	247	17.341	19.837	9.466	1.00	2.00
MOTA	1547	CE3	TRP	247	15.352	19.599	8.116	1.00	2.00
MOTA	1548	CD1	TRP	247	16.547	19.600	11.530	1.00	2.00
ATOM	1549	NE1	TRP	247	17.678	19.820	10.793	1.00	2.00
ATOM	1550	CZ2	TRP	247	18.145	20.018	8.339	1.00	2.00
MOTA	1551	CZ3	TRP	247	16.147	19.779	6.998	1.00	2.00
MOTA	1552	CH2	TRP	247	17.528	19.982	7.113	1.00	2.00
ATOM	1553	С	TRP	247	14.830	17.070	12.161	1.00	2.00
ATOM	1554	0	TRP	247	15.710	16.386	11.659	1.00	2.00
MOTA	1555	N	SER	248	14.767	17.327	13.463	1.00	10.46
MOTA	1556	CA	SER	248	15.744	16.804	14.417	1.00	10.46
ATOM	1557	CB	SER	248	15.475	17.351	15.836	1.00	2.00
ATOM	1558	OG	SER	248	15.486	18.772	15.908	1.00	2.00
MOTA	1559	C	SER	248	15.677	15.271	14.411	1.00	10.46
MOTA	1560	0	SER	248	16.712	14.605	14.460	1.00	2.00
ATOM	1561	N	VAL	249	14.464	14.723	14.304	1.00	6.38
ATOM	1562	CA	VAL	249	14.250	13.275	14.267	1.00	6.38
ATOM	1563	CB	VAL	249	12.728	12.902	14.189	1.00	2.90
MOTA	1564	CG1	VAL	249	12.550	11.404	14.200	1.00	2.90
MOTA	1565	CG2	LAV	249	11.948	13.520	15.342	1.00	2.90
ATOM	1566	C	VAL	249	14.970	12.667	13.050	1.00	6.38
ATOM	1567	0	VAL	249	15.586	11.606	13.150	1.00	2.90
ATOM	1568	N	GLY	250	14.906	13.357	11.914	1.00	2.00
MOTA	1569	CA	GLY	250	15.545	12.883	10.698	1.00	2.00
ATOM	1570	C	GTA	250	17.060	12.971	10.710	1.00	2.00
ATOM	1571	0	GLY	250	17.732	12.207	10.021	1.00	20.96
ATOM	1572	N	CYS	251	17.600	13.908	11.482	1.00	11.18
ATOM	1573	CA	CYS	251	19.047	14.109	11.597	1.00	11.18
MOTA	1574	CB	CYS	251	19.359	15.372	12.409	1.00	6.78
ATOM	1575	SG	CYS	251	19.017	16.935	11.612	1.00	6.78
MOTA	1576	С	CYS	251	19.623	12.934	12.336		11.18 6.78
MOTA	1577	0	CYS	251	20.796	12.594	12.177		22.98
MOTA	1578	N	ILE	252	18.784		13.196		22.98
MOTA	1579	CA		252	19.134		14.005		
ATOM	1580			252	18.260		15.274		2.00 2.00
MOTA	1581		2 ILE	252	18.472		15.970		2.00
MOTA	1582	CG:	1 ILE	252	18.583		16.199		
MOTA	1583	CD:	1 ILE	252	17.732				2.00
ATOM	1584	C	ILE	252	18.972				22.98
ATOM	1585	0	ILE	252	19.930				2.00
ATOM	1586	N	MET		17.783				2.00
MOTA	1587	CA	MET	253	17.538				2.00
MOTA	1588	CB		253	16.152			_	4.75
MOTA	1589	CG	MET	253	15.880			_	4.75
MOTA	1590	SD	MET	253	14.288			_	4.75
MOTA	1591	. CE	MET	253	14.189	6.019	8.680	1.00	4.75



## FIG. 3BB

		~	MERC	252	18.582	8.364	10.758	1.00	2.00
ATOM	1592	C	MET	253		7.264	10.436	1.00	4.75
MOTA	1593	0	MET	253	19.000	9.490	10.189	1.00	4.43
MOTA	1594	N	GLY	254	18.996		9.136	1.00	4.43
MOTA	1595	CA	GLY	254	19.992	9.481		1.00	4.43
MOTA	1596	C	GLY	254	21.359	9.089	9.655	1.00	19.89
MOTA	1597	0	GLY	254	22.172	8.552	8.915		26.96
MOTA	1598	N	GLU	255	21.605	9.360	10.933	1.00	
MOTA	1599	CA	GLU	255	22.863	9.030	11.599	1.00	26.96
MOTA	1600	CB	GLU	255	23.051	9.943	12.817	1.00	19.79
MOTA	1601	CG	GLU	255	24.434	9.872	13.477	1.00	19.79
MOTA	1602	CD	GLU	255	24.713	11.057	14.392	1.00	19.79
MOTA	1603	OE1	${ t GLU}$	255	23.824	11.922	14.531	1.00	19.79
MOTA	1604	OE2	GLU	255	25.821	11.136	14.952	1.00	19.79
MOTA	1605	C	GLU	255	22.872	7.551	12.017	1.00	26.96
ATOM	1606	0	GLU	255	23.920	6.903	11.997	1.00	19.79
MOTA	1607	N	MET	256	21.697	7.020	12.359	1.00	22.99
MOTA	1608	CA	MET	256	21.554	5.615	12.746	1.00	22.99
ATOM	1609	CB	MET	256	20.112	5.311	13.217	1.00	4.42
ATOM	1610	CG	MET	256	19.741	5.871	14.594	1.00	4.42
ATOM	1611	SD	MET	256	17.982	5.762	15.032	1.00	4.42
ATOM	1612	CE	MET	256	17.978	4.420	16.092	1.00	4.42
ATOM	1613	C	MET	256	21.873	4.754	11.514	1.00	22.99
ATOM	1614	ō	MET	256	22.243	3.586	11.636	1.00	4.42
MOTA	1615	N	VAL	257	21.744	5.358	10.336	1.00	2.00
MOTA	1616	CA	VAL	257	21.982	4.700	9.057	1.00	2.00
ATOM	1617	CB	VAL	257	20.998	5.237	7.975	1.00	9.27
ATOM	1618		VAL	257	21.367	4.728	6.585	1.00	9.27
	1619		VAL	257	19.580	4.853	8.327	1.00	9.27
ATOM	1620	C	VAL	257	23.403	4.929	8.554	1.00	2.00
ATOM		0	VAL	257	24.148	3.987	8.291	1.00	9.27
MOTA	1621		ARG	258	23.765	6.197	8.409	1.00	14.20
ATOM	1622	N	ARG	258	25.076	6.575	7.907	1.00	14.20
ATOM	1623	CA	ARG	258	25.073	8.020	7.391	1.00	18.38
MOTA	1624	CB	ARG	258	25.598	8.182	6.001	1.00	18.38
ATOM	1625	CG		258	24.941	9.313	5.239	1.00	18.38
ATOM	1626	CD	ARG		25.581	10.606	5.471	1.00	18.38
MOTA	1627	NE	ARG	258	25.359	11.703	4.740	1.00	18.38
MOTA	1628	CZ	ARG	258	24.515	11.676	3.714	1.00	18.38
ATOM	1629		ARG	258	25.963	12.844	5.055	1.00	18.38
ATOM	1630		ARG	258		6.398	8.926	1.00	14.20
MOTA	1631	C	ARG	258	26.196	6.369	8.566	1.00	18.38
MOTA	1632	0	ARG	258	27.369	6.243	10.195	1.00	6.43
MOTA	1633	N	HIS	259	25.828		11.269	1.00	6.43
MOTA	1634	CA	HIS	259	26.805	6.088	11.163	1.00	14.61
MOTA	1635	CB	HIS	259	27.510	4.740		1.00	14.61
MOTA	1636	CG	HIS	259	26.601	3.576	11.387	1.00	14.61
MOTA	1637		HIS	259	26.413	2.445	10.665		14.61
ATOM	1638		HIS	259	25.714	3.510	12.438	1.00	14.61
MOTA	1639		HIS	259	25.023	2.396	12.362	1.00	14.61
MOTA	1640		HIS	259	25.423	1.727	11.293	1.00	
ATOM	1641	C	HIS	259	27.809	7.230	11.294	1.00	6.43
ATOM	1642	0	HIS	259	28.983	7.059	11.643	1.00	14.61
MOTA	1643	N	LYS	260	27.326	8.391	10.869	1.00	7.67
ATOM	1644	CA	LYS	260	28.085	9.627	10.848	1.00	7.67
MOTA	1645	CB	LYS	260	28.850	9.789	9.530	1.00	21.52
MOTA	1646	CG	LYS	260	30.252	9.148	9.536	1.00	21.52
MOTA	1647	CD	LYS	260	31.112	9.537	8.315	1.00	21.52
MOTA	1648	CE	LYS	260	30.605		7.012	1.00	21.52
MOTA	1649	NZ	LYS	260	31.486		5.853	1.00	21.52
ATOM	1650	C	LYS	260	27.043	10.723	11.024	1.00	7.67



## FIG. 3CC

ATOM	1651	0	LYS	260	25.866	10.520	10.691	1.00	21.52
MOTA	1652	N	ILE	261	27.437	11.838	11.638	1.00	2.00
MOTA	1653	CA	ILE	261	26.515	12.950	11.844	1.00	2.00
ATOM	1654	CB	ILE	261	27.091	14.053	12.767	1.00	15.02
MOTA	1655	CG2	ILE	261	25.959	14.937	13.284	1.00	15.02
MOTA	1656	CG1	ILE	261	27.848	13.462	13.960	1.00	15.02
MOTA	1657	CD1	ILE	261	28.606	14.516	14.778	1.00	15.02
ATOM	1658	C	ILE	261	26.306	13.575	10.475	1.00	2.00
MOTA	1659	0	ILE	261	27.271	13.922	9.798	1.00	15.02
MOTA	1660	N	LEU	262	25.047	13.726	10.081	1.00	22.16
MOTA	1661	CA	LEU	262	24.700	14.298	8.777	1.00	22.16
MOTA	1662	CB	LEU	262	23.187	14.270	8.605	1.00	12.98
ATOM	1663	CG	LEU	262	22.463	12.931	8.609	1.00	12.98
ATOM	1664	CD1	LEU	262	21.008	13.190	8.267	1.00	12.98
ATOM	1665	CD2	LEU	262	23.091	12.011	7.588	1.00	12.98
MOTA	1666	С	LEU	262	25.237	15.724	8.471	1.00	22.16
MOTA	1667	0	LEU	262	25.986	15.922	7.498	1.00	12.98
MOTA	1668	N	PHE	263	24.841	16.707	9.280	1.00	2.00
ATOM	1669	CA	PHE	263	25.275	18.100	9.085	1.00	2.00
MOTA	1670	CB	PHE	263	24.065	19.009	8.802	1.00	7.82
ATOM	1671	CG	PHE	263	22.949	18.344	8.049	1.00	7.82
ATOM	1672		PHE	263	23.136	17.886	6.752	1.00	7.82
ATOM	1673	CD2	PHE	263	21.693	18.203	8.640	1.00	7.82
ATOM	1674		PHE	263	22.092	17.288	6.045	1.00	7.82
MOTA	1675	CE2		263	20.639	17.609	7.950	1.00	7.82
ATOM	1676	CZ	PHE	263	20.836	17.151	6.645	1.00	7.82
ATOM	1677	C	PHE	263	26.037	18.718	10.275	1.00	2.00
ATOM	1678	ō	PHE	263	25,507	19.592	10.956	1.00	7.82
ATOM	1679	N	PRO	264	27.296	18.305	10.516	1.00	18.59
ATOM	1680	CD	PRO	264	28.074	17.296	9.787	1.00	14.60
ATOM	1681	CA	PRO	264	28.076	18.857	11.636	1.00	18.59
ATOM	1682	CB	PRO	264	29.412	18.102	11.540	1.00	14.60
ATOM	1683	CG	PRO	264	29.493	17.689	10.112	1.00	14.60
ATOM	1684	C	PRO	264	28.234	20.406	11.663	1.00	18.59
ATOM	1685	Ö	PRO	264	27.384	21.096	12.223	1.00	14.60
ATOM	1686	N	GLY	265	29.324	20.942	11.100	1.00	26.76
ATOM	1687	CA	GLY	265	29.525	22.387	11.085	1.00	26.76
ATOM	1688	C	GLY	265	29.901	23.014	12.425	1.00	26.76
ATOM	1689	ō	GLY	265	29.130	22.947	13.381	1.00	2.00
ATOM	1690	N	ARG	266	31.090	23.622	12.487	1.00	2.58
ATOM	1691	CA	ARG	266	31.630	24.273	13.687	1.00	2.58
ATOM	1692	CB	ARG	266	32.986	24.918	13.394	1.00	31.96
ATOM	1693	CG	ARG	266	33.982	24.111	12.570	1.00	31.96
ATOM	1694	CD	ARG	266	34.966	25.050	11.846	1.00	31.96
ATOM	1695	NE	ARG	266	34.293	25.983	10.928	1.00	31.96
ATOM	1696	CZ	ARG	266	34.322	27.317	11.024	1.00	31.96
ATOM	1697		L ARG	266	34.995	27.922	12.003	1.00	31.96
ATOM	1698		2 ARG	266	33.678	28.057	10.127	1.00	31.96
MOTA	1699	C	ARG	266	30.744	25.388	14.224	1.00	2.58
ATOM	1700	Õ	ARG	266	30.895	25.791	15.375	1.00	31.96
ATOM	1701	N	ASP	267	29.913	25.963	13.359	1.00	30.47
ATOM	1701	CA	ASP	267	29.020	27.052	13.754		30.47
	1702	CB	ASP	267	29.768		13.752		28.71
ATOM		CG		267	30.417		12.404		28.71
MOTA	1704		ASP	267	31.125		11.841		28.71
ATOM	1705		2 ASP	267	30.237		11.909		28.71
MOTA	1706		ASP ASP	267 267	27.827		12.814		30.47
MOTA	1707		ASP		27.927	_			28.71
ATOM	1708								13.24
ATOM	1709	N	TYR	268	26.761	21.133			

### FIG. 3DD

ATOM	1710	CA	TYR	268	25.538	27.933	12.455	1.00	13.24
ATOM	1711	CB	TYR	268	24.605	29.009	13.023	1.00	26.47
ATOM	1712	CG	TYR	268	23.570	28.524	14.025	1.00	26.47
ATOM	1713	CD1	TYR	268	23.432	27.170	14.343	1.00	26.47
ATOM	1714	CE1	TYR	268	22.499	26.737	15.321	1.00	26.47
ATOM	1715	CD2	TYR	268	22.750	29.432	14.692	1.00	26.47
ATOM	1716	CE2	TYR	268	21.820	29.012	15.663	1.00	26.47
ATOM	1717	CZ	TYR	268	21.700	27.668	15.978	1.00	26.47
ATOM	1718	OH	TYR	268	20.804	27.293	16.968	1.00	26.47
ATOM	1719	C	TYR	268	25.842	28.275	11.004	1.00	13.24
ATOM	1720	ŏ	TYR	268	25.073	27.934	10.121	1.00	26.47
ATOM	1721	N	ILE	269	26.969	28.932	10.750	1.00	27.51
ATOM	1722	CA	ILE	269	27.340	29.299	9.383	1.00	27.51
ATOM	1723	CB	ILE	269	28.529	30.302	9.351	1.00	26.87
	1724	CG2	ILE	269	28.970	30.546	7.911	1.00	26.87
ATOM	1725	CG1	ILE	269	28.165	31.601	10.073	1.00	26.87
ATOM	1726	CD1		269	26.945	32.267	9.541	1.00	26.87
MOTA		CDI	ILE	269	27.790	28.055	8.633	1.00	27.51
ATOM	1727				27.790	27.754	7.547	1.00	26.87
MOTA	1728	0	ILE	269	28.758	27.369	9.231	1.00	5.20
MOTA	1729	N	ASP	270		26.161	8.692	1.00	5.20
MOTA	1730	CA	ASP	270	29.347		9.617	1.00	33.24
ATOM	1731	CB	ASP	270	30.495	25.750		1.00	33.24
MOTA	1732	CG	ASP	270	31.302	24.588	9.078		33.24
MOTA	1733		ASP	270	31.141	24.228	7.891	1.00	
MOTA	1734		ASP	270	32.119	24.025	9.838	1.00	33.24 5.20
ATOM	1735	С	ASP	270	28.304	25.045	8.624	1.00	
MOTA	1736	0	ASP	270	28.338	24.183	7.746	1.00	33.24
MOTA	1737	N	GLN	271	27.351	25.093	9.543	1.00	25.51
MOTA	1738	CA	GLN	271	26.307	24.086	9.643	1.00	25.51
MOTA	1739	CB	GLN	271	25.621	24.244	10.990	1.00	9.91
MOTA	1740	CG	GLN	271	25.393	22.960	11.713	1.00	9.91
MOTA	1741	CD	GLN	271	23.953	22.572	11.694	1.00	9.91
ATOM	1742		GLN	271	23.133	23.178	12.380	1.00	9.91
MOTA	1743	NE2	GLN	271	23.623	21.567	10.904	1.00	9.91
MOTA	1744	C	GLN	271	25.290	24.156	8.515	1.00	25.51
MOTA	1745	0	GLN	271	24.834	23.130	8.025	1.00	9.91
ATOM	1746	N	TRP	272	24.920	25.371	8.129	1.00	2.00
ATOM	1747	CA	TRP	272	23.961	25.582	7.059	1.00	2.00
ATOM	1748	CB	TRP	272	23.501	27.034	7.055	1.00	2.00
ATOM	1749	CG	TRP	272	22.639	27.413	5.902	1.00	2.00
ATOM	1750	CD2	TRP	272	21.261	27.040	5.670	1.00	2.00
ATOM	1751	CE2	TRP	272	20.849	27.675	4.487	1.00	2.00
ATOM	1752	CE3	TRP	272	20.353	26.236	6.366	1.00	2.00
ATOM	1753	CD1	TRP	272	22.982	28.232	4.862	1.00	2.00
ATOM	1754	NE1	TRP	272	21.915	28.395	4.012	1.00	2.00
ATOM	1755	CZ2	TRP	272	19.550	27.524	3.966	1.00	2.00
ATOM	1756		TRP	272	19.068	26.088	5.851	1.00	2.00
ATOM	1757	CH2	TRP	272	18.676	26.732	4.665	1.00	2.00
ATOM	1758	C	TRP	272	24.600	25.214	5.726	1.00	2.00
ATOM	1759	ō	TRP	272	23.912	24.844	4.769	1.00	2.00
ATOM	1760	N	ASN	273	25.927	25.299	5.683	1.00	9.70
ATOM	1761	CA	ASN	273	26.686	24.971	4.489	1.00	9.70
ATOM	1762	CB	ASN	273	28.162	25.319	4.672	1.00	18.64
ATOM	1763	CG	ASN	273	28.395	26.809	4.841	1.00	18.64
ATOM	1764		. ASN	273	29.434	27.219	5.338	1.00	18.64
ATOM	1765		ASN	273	27.430	27.627	4.423	1.00	18.64
ATOM	1766	C	ASN	273	26.532	23.493	4.208	1.00	9.70
ATOM	1767	0	ASN	273	26.176	23.100	3.098	1.00	18.64
ATOM		N	LYS	273 274	26.704	22.685	5.247	1.00	3.97
ATOM	1768	1/4	шы	4/4	20.704	22.005	3.2.7		J.2.



## FIG. 3EE

MOTA	1769	CA	LYS	274	26.578	21.239	5.140	1.00	3.97
ATOM	1770	CB	LYS	274	26.883	20.593	6.491	1.00	14.41
ATOM	1771	CG	LYS	274	28.160	21.077	7.123	1.00	14.41
ATOM	1772	CD	LYS	274	29.332	20.845	6.200	1.00	14.41
ATOM	1773	CE	LYS	274	29.818	19.414	6.283	1.00	14.41
MOTA	1774	NZ	LYS	274	30.453	19.182	7.591	1.00	14.41
MOTA	1775	С	LYS	274	25.167	20.838	4.701	1.00	3.97
ATOM	1776	0	LYS	274	25.002	19.940	3.880	1.00	14.41
MOTA	1777	N	VAL	275	24.161	21.537	5.224	1.00	11.35
MOTA	1778	CA	VAL	275	22.754	21.272	4.922	1.00	11.35 13.06
MOTA	1779	CB	VAL	275	21.819	22.227	5.715	1.00	13.06
MOTA	1780	CG1	VAL	275	20.365	22.029	5.313	1.00 1.00	13.06
ATOM	1781		VAL	275	21.993	21.993	7.191 3.446	1.00	11.35
MOTA	1782	C	VAL	275	22.410	21.417	2.877	1.00	13.06
MOTA	1783	0	VAL	275	21.724	20.569 22.523	2.851	1.00	34.01
MOTA	1784	N	ILE	276	22.852	22.803	1.446	1.00	34.01
MOTA	1785	CA	ILE	276	22.595 22.666	24.326	1.152	1.00	6.67
MOTA	1786	CB	ILE	276		25.023	1.810	1.00	6.67
ATOM	1787		ILE	276	21.498 24.022	24.894	1.595	1.00	6.67
MOTA	1788		ILE ILE	276 276	24.279	26.346	1.194	1.00	6.67
ATOM	1789		ILE	276 276	23.550	23.340	0.529	1.00	34.01
MOTA	1790	C	ILE	276	23.224	21.748	-0.618	1.00	6.67
ATOM	1791 1792	N O	GLU	277	24.706	21.670	1.061	1.00	2.00
MOTA MOTA	1792	CA	GLU	277	25.694	20.930	0.302	1.00	2.00
ATOM	1794	CB	GLU	277	26.978	20.857	1.110	1.00	11.08
ATOM	1795	CG	GLU	277	28.227	20.945	0.298	1.00	11.08
ATOM	1796	CD	GLU	277	29.395	20.231	0.959	1.00	11.08
MOTA	1797		GLU	277	29.651	20.473	2.171	1.00	11.08
ATOM	1798		GLU	277	30.043	19.407	0.263	1.00	11.08
ATOM	1799	C	GLU	277	25.207	19.508	-0.002	1.00	2.00
ATOM	1800	ō	GLU	277	25.833	18.784	-0.767	1.00	11.08
MOTA	1801	N	GLN	278	24.101	19.108	0.622	1.00	7.26
ATOM	1802	CA	GLN	278	23.533	17.775	0.450	1.00	7.26
ATOM	1803	CB	GLN	278	23.559	17.012	1.768	1.00	6.70
MOTA	1804	CG	GLN	278	24.939	16.832	2.353	1.00	6.70
ATOM	1805	CD	GLN	278	24.913	16.050	3.640	1.00	6.70
MOTA	1806	OE1	GLN	278	24.207	15.048	3.752	1.00	6.70
MOTA	1807	NE2		278	25.689	16.499	4.625	1.00	6.70
ATOM	1808	С	GLN	278	22.108	17.799	-0.054	1.00	7.26
ATOM	1809	0	GLN	278	21.830	17.340	-1.138	1.00	6.70
MOTA	1810	N	PEA	279	21.198	18.328	0.743	1.00	20.28
MOTA	1811	CA	LEU	279	19.796	18.364	0.352	1.00	20.28 12.10
MOTA	1812	CB	LEU	279	18.901	18.628	1.581	1.00 1.00	12.10
MOTA	1813	CG	LEU	279	19.274	18.001	2.944 3.985	1.00	12.10
MOTA	1814		LEU	279	18.256	18.392	2.881	1.00	12.10
MOTA	1815		FEU	279	19.386	16.480 19.393	-0.769	1.00	20.28
ATOM	1816	C	LEU	279	19.550 18.573	19.393	-1.511	1.00	12.10
MOTA	1817	0	LEU	279	20.467	20.354	-0.913	1.00	2.00
MOTA	1818	N	GLY	280 280	20.467	21.385	-1.941	1.00	2.00
MOTA MOTA	1819	CA	GLY GLY	280	19.768	22.717	-1.489	1.00	2.00
	1820	C		280	19.066	22.779	-0.482	1.00	11.83
ATOM ATOM	1821 1822	N O	GLY THR	281	20.046	23.787	-2.231	1.00	2.00
ATOM	1822	CA	THR	281	19.549	25.737	-1.917	1.00	2.00
MOTA	1824	CB	THR		20.145	26.205	-2.923	1.00	13.34
ATOM	1825	OG1			21.582	26.144	-2.906	1.00	13.34
ATOM	1826	CG2			19.701	27.628	-2.573	1.00	13.34
ATOM	1827	C	THR		17.999	25.181	-1.922	1.00	2.00
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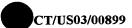
## FIG. 3FF

MOTA	1828	0	THR	281	17.374	24.830	-2.920	1.00	13.34
ATOM	1829	N	PRO	282	17.375	25.631	-0.811	1.00	17.13
MOTA	1830	CD	PRO	282	17.997	26.220	0.386	1.00	3.54
MOTA	1831	CA	PRO	282	15.910	25.707	-0.698	1.00	17.13
MOTA	1832	CB	PRO	282	15.708	26.350	0.673	1.00	3.54
ATOM	1833	CG	PRO	282	16.915	27.164	0.859	1.00	3.54
MOTA	1834	C	PRO	282	15.172	26.484	-1.787	1.00	17.13
ATOM	1835	0	PRO	282	15.706	27.440	-2.357	1.00	3.54
MOTA	1836	N	CYS	283	13.934	26.072	-2.059	1.00	2.45
MOTA	1837	CA	CYS	283	13.110	26.728	-3.060	1.00	2.45
MOTA	1838	CB	CYS	283	11.796	25.953	-3.298	1.00	32.82
ATOM	1839	SG	CYS	283	10.506	26.042	-1.999	1.00	32.82
MOTA	1840	C	CYS	283	12.835	28.175	-2.664	1.00	2.45
MOTA	1841	0	CYS	283	12.799	28.512	-1.488	1.00	32.82
MOTA	1842	N	PRO	284	12.705	29.059	-3.658	1.00	29.31
MOTA	1843	CD	PRO	284	12.845	28.755	-5.094	1.00	30.81
MOTA	1844	CA.	PRO	284	12.442	30.486	-3.464	1.00	29.31
MOTA	1845	CB	PRO	284	12.120	30.948	-4.885	1.00	30.81
MOTA	1846	CG	PRO	284	13.079	30.125	-5.696	1.00	30.81
ATOM	1847	C	PRO	284	11.324	30.801	-2.467	1.00	29.31
ATOM	1848	0	PRO	284	11.454	31.734	-1.667	1.00	30.81
MOTA	1849	N	ALA	285	10.251	30.008	-2.486	1.00	17.96
MOTA	1850	CA	ALA	285	9.144	30.230	-1.572	1.00	17.96
MOTA	1851	CB	ALA	285	8.084	29.158	-1.767	1.00	9.64
ATOM	1852	С	ALA	285	9.679	30.246	-0.124	1.00	17.96
ATOM	1853	0	ALA	285	9.308	31.119	0.660	1.00	9.64
ATOM	1854	N	PHE	286	10.630	29.358	0.176	1.00	4.52
ATOM	1855	CA	PHE	286	11.236	29.277	1.502	1.00	4.52
MOTA	1856	CB	PHE	286	12.185	28.079	1.578	1.00	4.64
MOTA	1857	CG	PHE	286	12.941	27.992	2.878	1.00	4.64
ATOM	1858	CD1	PHE	286	12.324	27.494	4.019	1.00	4.64
MOTA	1859	CD2	PHE	286	14.269	28.412	2.958	1.00	4.64
ATOM	1860	CE1	PHE	286	13.014	27.412	5.228	1.00	4.64
MOTA	1861	CE2	PHE	286	14.976	28.339	4.158	1.00	4.64
ATOM	1862	CZ	PHE	286	14.351	27.839	5.299	1.00	4.64
MOTA	1863	C	PHE	286	11.982	30.565	1.871	1.00	4.52
ATOM	1864	0	PHE	286	11.848	31.067	2.997	1.00	4.64
MOTA	1865	N	MET	287	12.748	31.100	0.915	1.00	19.98
ATOM	1866	CA	MET	287	13.511	32.333	1.097	1.00	19.98
MOTA	1867	CB	MET	287	14.371	32.602	-0.131	1.00	23.24
MOTA	1868	CG	MET	287	15.853	32.633	0.139	1.00	23.24
MOTA	1869	SD	MET	287	16.574	30.987	0.341	1.00	23.24
ATOM	1870	CE	MET	287	17.149	30.610	-1.343	1.00	23.24
ATOM	1871	C	MET	287	12.569	33.516	1.327	1.00	19.98
MOTA	1872	0	MET	287	12.876	34.423	2.114	1.00	23.24
ATOM	1873	N	LYS	288	11.419	33.493	0.657	1.00	9.91
MOTA	1874	CA	LYS	288	10.433	34.547	0.805	1.00	9.91
ATOM	1875	CB	LYS	288	9.204	34.256	-0.057	1.00	54.51
MOTA	1876	CG	LYS	288	9.363	34.698	-1.501	1.00	54.51
MOTA	1877	CD	LYS	288	8.116	34.431	-2.319	1.00	54.51
MOTA	1878	CE	LYS	288	8.376	34.747	-3.776	1.00	54.51
MOTA	1879	NZ	LYS	288	7.226	34.380	-4.654	1.00	54.51
MOTA	1880	C	LYS	288	10.021	34.703	2.259	1.00	9.91
MOTA	1881	0	LYS	288	9.599	35.778	2.680	1.00	54.51
MOTA	1882	N	LYS	289	10.180	33.631	3.028	1.00	48.86
MOTA	1883	CA	LYS	289	9.829	33.628	4.450	1.00	48.86
MOTA	1884	CB	LYS	289	9.502	32.196	4.896	1.00	28.25
MOTA	1885	CG	LYS	289	8.343	31.538	4.169	1.00	28.25
MOTA	1886	CD	LYS	289	8.255	30.064	4.554	1.00	28.25
				•					



## FIG. 3GG

ATOM	1887	CE	LYS	289		6.927	29.444	4.131	1.00	28.25
MOTA	1888		LYS	289		6.843	28.016	4.540	1.00	28.25
ATOM	1889		LYS	289	1	.0.949	34.195	5.351	1.00	48.86
ATOM	1890		LYS	289	1	.0.723	34.521	6.519	1.00	28.25
ATOM	1891		LEU	290	1	2.143	34.336	4.791	1.00	16.09
ATOM	1892	CA	LEU	290	1	L3.290	34.822	5.547	1.00	16.09
MOTA	1893	CB	LEU	290		L4.585	34.379	4.870	1.00	23.78
MOTA	1894	CG	LEU	290	1	L4.680	32.948	4.334	1.00	23.78
ATOM	1895	CD1	LEU	290		L5.998	32.748	3.571	1.00	23.78
ATOM	1896	CD2	LEU	290	1	L4.535	31.958	5.498	1.00	23.78 16.09
ATOM	1897	С	LEU	290		13.326	36.334	5.702	1.00	23.78
MOTA	1898	0	LEU	290		13.092	37.053	4.736	1.00	23.76
MOTA	1899	N	GLN	291		13.631	36.815	6.912	1.00	22.36
ATOM	1900	CA	GLN	291		13.741	38.257	7.177	1.00	39.09
MOTA	1901	CB	GLN	291		14.099	38.514	8.651	1.00	39.09
MOTA	1902	CG	GLN	291		14.582	39.946	8.993	1.00	39.09
MOTA	1903	CD	GLN	291		13.469	41.005	9.052	1.00	39.09
MOTA	1904	OE1	GLN	291		12.300	40.730	8.741	1.00	39.09
ATOM	1905	NE2	GLN	291		13.841	42.229	9.445	1.00	22.36
MOTA	1906	С	GLN	291		14.834	38.788	6.253	1.00 1.00	39.09
ATOM	1907	0	GLN	291		15.871	38.163	6.085	1.00	11.17
ATOM	1908	N	PRO	292		14.603	39.946	5.634	1.00	16.09
ATOM	1909	CD	PRO	292		13.414	40.780	5.878	1.00	11.17
ATOM	1910	CA	PRO	292		15.517	40.619	4.703	1.00	16.09
MOTA	1911	CB	PRO	292		15.015	42.058	4.739	1.00	16.09
MOTA	1912	CG	PRO	292		13.542	41.867	4.834 4.998	1.00	11.17
MOTA	1913	C	PRO	292		17.012	40.530		1.00	16.09
MOTA	1914	0	PRO	292		17.811	40.364	4.078 6.266	1.00	4.79
MOTA	1915	N	THR	293		17.393	40.618	6.611	1.00	4.79
MOTA	1916	CA	THR	293		18.810	40.573	7.945	1.00	13.45
ATOM	1917	CB	THR	293		19.140	41.301 41.251	8.170	1.00	13.45
MOTA	1918	OG1		293		20.558	40.668	9.117	1.00	13.45
MOTA	1919	CG2		293		18.408	39.166	6.640	1.00	4.79
MOTA	1920	C	THR	293		19.363		6.577	1.00	13.45
MOTA	1921	0	THR	293		20.577		6.770	1.00	44.45
MOTA	1922	N	VAL	294		18.467 18.822		6.790	1.00	44.45
MOTA	1923	CA	VAL	294		17.930		7.779	1.00	21.86
MOTA	1924	CB	VAL	294		18.343		7.801	1.00	21.86
MOTA	1925		LVAL	294		18.022		9.172	1.00	21.86
MOTA	1926	CG2		294		18.624		5.383	1.00	44.45
MOTA	1927	C	VAL	294		19.312		4.984	1.00	21.86
MOTA	1928	0	VAL	29 <b>4</b> 295		17.686		4.642	1.00	2.00
MOTA	1929	N	ARG ARG			17.369		3.274	1.00	2.00
ATOM	1930			295 295		16.106		2.794		35.93
MOTA	1931	CB	ARG	295 295		15.364		1.664		35.93
MOTA	1932	CG	ARG ARG	295 295		14.280		1.010		35.93
ATOM	1933	CD		295 295	•	13.376		1.980		35.93
MOTA	1934			295		12.132		1.717		35.93
MOTA	1935		1 ARG	295		11.610		0.499		35.93
ATOM	1936		2 ARG	295		11.418		2.675		35.93
MOTA	1937	_	ARG	295		18.544		2.381		2.00
MOTA	1938	_	ARG	295		18.81		1.378		35.93
ATOM	1939		ASN	296		19.26		2.783		23.98
MOTA	1940 1941			296 296		20.41		2.031		23.98
MOTA	1941			296		20.92		2.600		20.87
ATOM	1942			296		21.62		1.560		20.87
MOTA	1943		1 ASN			20.98		0.865		20.87
ATOM ATOM	1944		2 ASN			22.92		1.371		20.87
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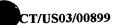
## FIG. 3HH

							0 000	1 00	22 00
MOTA	1946	C	ASN	296	21.553	37.299	2.066	1.00	23.98
ATOM	1947	0	ASN	296	22.239	37.097	1.068	1.00	20.87
ATOM	1948	N	TYR	297	21.765	36.710	3.238	1.00	14.54
ATOM	1949	CA	TYR	297	22.823	35.738	3.463	1.00	14.54
ATOM	1950	CB	TYR	297	22.878	35.396	4.955	1.00	12.06
ATOM	1951	CG	TYR	297	23.853	34.309	5.295	1.00	12.06
ATOM	1952	CD1		297	25.221	34.513	5.171	1.00	12.06
ATOM	1953	CE1	TYR	297	26.133	33.509	5.481	1.00	12.06
	1954	CD2	TYR	297	23.411	33.070	5.739	1.00	12.06
MOTA		CE2	TYR	297	24.318	32.056	6.050	1.00	12.06
ATOM	1955			297	25.678	32.284	5.918	1.00	12.06
ATOM	1956	CZ	TYR		26.579	31.288	6.223	1.00	12.06
MOTA	1957	ОН	TYR	297		34.464	2.648	1.00	14.54
ATOM	1958	C	TYR	297	22.646		1.941	1.00	12.06
MOTA	1959	0	TYR	297	23.561	34.036	2.747	1.00	4.63
MOTA	1960	N	VAL	298	21.449	33.892			4.63
MOTA	1961	CA	VAL	298	21.088	32.656	2.077	1.00	
MOTA	1962	CB	VAL	298	19.723	32.124	2.581	1.00	42.51
MOTA	1963	CG1	VAL	298	19.304	30.882	1.785	1.00	42.51
ATOM	1964	CG2	VAL	298	19.790	31.802	4.064	1.00	42.51
MOTA	1965	C	VAL	298	21.010	32.784	0.565	1.00	4.63
ATOM	1966	0	VAL	298	21.485	31.898	-0.163	1.00	42.51
ATOM	1967	N	GLU	299	20.388	33.859	0.080	1.00	21.61
ATOM	1968	CA	GLU	299	20.264	34.064	-1.361	1.00	21.61
ATOM	1969	CB	GLU	299	19.329	35.220	-1.671	1.00	40.37
	1970	CG	GLU	299	17.884	34.920	-1.312	1.00	40.37
MOTA	1971	CD	GLU	299	16.986	36.142	-1.378	1.00	40.37
MOTA			GLU	299	17.464	37.260	-1.076	1.00	40.37
ATOM	1972				15.802	35.984	-1.722	1.00	40.37
ATOM	1973		GLU	299	21.632	34.301	-1.973	1.00	21.61
ATOM	1974	C	GLU	299		33.735	-3.015	1.00	40.37
ATOM	1975	0	GLU	299	21.957			1.00	5.94
MOTA	1976	N	ASN	300	22.455	35.104	-1.310		5.94
MOTA	1977	CA	ASN	300	23.790	35.372	-1.818	1.00	39.13
MOTA	1978	CB	ASN	300	24.185	36.816	-1.512	1.00	
MOTA	1979	CG	ASN	300	23.274	37.827	-2.201	1.00	39.13
ATOM	1980	OD1	. ASN	300	23.558	38.274	-3.314	1.00	39.13
MOTA	1981	ND2	ASN	300	22.163	38.168	-1.558	1.00	39.13
ATOM	1982	C	ASN	300	24.743	34.356	-1.193	1.00	5.94
ATOM	1983	0	ASN	300	25.658	34.706	-0.441	1.00	39.13
MOTA	1984	N	ARG	301	24.494	33.087	-1.505	1.00	26.43
ATOM	1985	CA	ARG	301	25.280	31.956	-1.005	1.00	26.43
ATOM	1986	СВ	ARG	301	24.505	31.286	0.153	1.00	45.38
ATOM	1987	CG	ARG	301	25.323	30.477	1.138	1.00	45.38
ATOM	1988	CD	ARG	301	25.484	31.225	2.445	1.00	45.38
ATOM	1989	NE	ARG	301	26.760		3.071	1.00	45.38
MOTA	1990	CZ	ARG	301	27.869		2.959	1.00	45.38
ATOM	1991		L ARG	301	27.870		2.249	1.00	45.38
			2 ARG	301	29.001		3.510	1.00	45.38
ATOM	1992			301	25.469		-2.158	1.00	26.43
MOTA	1993	C	ARG		24.525		-2.903	1.00	45.38
MOTA	1994	0	ARG	301			-2.315	1.00	7.81
MOTA	1995	N	PRO	302	26.684		-1.414	1.00	9.65
ATOM	1996	CD	PRO	302	27.840				7.81
ATOM	1997	CA	PRO	302	26.953		-3.387	1.00	9.65
MOTA	1998	CB	PRO	302	28.326		-3.009	1.00	
MOTA	1999	CG	PRO	302	28.420		-1.534	1.00	9.65
ATOM	2000	C	PRO	302	25.885		-3.432	1.00	7.81
MOTA	2001	0	PRO	302	25.600		-2.419	1.00	9.65
MOTA	2002	N	LYS	303	25.279		-4.604		38.56
MOTA	2003	CA	_	303	24.195	27.191	-4.785		38.56
ATOM	2004				23.260	27.627	-5.923	1.00	37.34
	<b>-</b>								



## FIG. 3II

							00 000	E 637	1.00	37.34
MOTA	2005		LYS	303		22.529	28.920	-5.637	1.00	37.34
ATOM	2006	CD	LYS	303		21.645	29.313	-6.794		37.34
MOTA	2007	CE	LYS	303		21.230	30.779	-6.697	1.00	
ATOM	2008	NZ	LYS	303		20.640	31.268	-7.995	1.00	37.34
MOTA	2009	C	LYS	303		24.587	25.738	-4.989	1.00	38.56
ATOM	2010		LYS	303		25.719	25.429	-5.367	1.00	37.34
ATOM	2011	N	TYR	304		23.626	24.859	-4.692	1.00	20.93
ATOM	2012	CA	TYR	304		23.768	23.405	-4.834	1.00	20.93
MOTA	2013	CB	TYR	304		24.093	22.741	-3.501	1.00	13.21
	2013	CG	TYR	304		25.503	22.977	-3.082	1.00	13.21
MOTA		CD1	TYR	304		26.536	22.201	-3.585	1.00	13.21
ATOM	2015		TYR	304		27.853	22.469	-3.252	1.00	13.21
MOTA	2016	CE1				25.814	24.013	-2.219	1.00	13.21
MOTA	2017	CD2	TYR	304		27.120	24.291	-1.876	1.00	13.21
MOTA	2018	CE2	TYR	304				-2.391	1.00	13.21
ATOM	2019	CZ	TYR	304		28.141	23.522	-2.075	1.00	13.21
MOTA	2020	OH	TYR	304		29.441	23.858		1.00	20.93
ATOM	2021	С	TYR	304		22.492	22.796	-5.388		13.21
MOTA	2022	0	TYR	304		21.395	23.037	-4.878	1.00	
MOTA	2023	N	ALA	305		22.645	22.006	-6.446	1.00	21.50
MOTA	2024	CA	ALA	305		21.513	21.354	-7.096	1.00	21.50
MOTA	2025	CB	ALA	305		21.991	20.549	-8.290	1.00	20.54
MOTA	2026	С	ALA	305		20.815	20.454	-6.102	1.00	21.50
ATOM	2027	0	ALA	305		19.593	20.350	-6.103	1.00	20.54
ATOM	2028	N	GLY	306		21.613	19.836	-5.230	1.00	20.44
ATOM	2029	CA	GLY	306		21.093	18.937	-4.213	1.00	20.44
ATOM	2030	C	GLY	306		21.169	17.482	-4.628	1.00	20.44
	2030	Ö	GLY	306		20.868	17.134	-5.778	1.00	20.50
ATOM			LEU	307		21.615	16.640	-3.703	1.00	6.20
ATOM	2032	N		307		21.729	15.209	-3.939	1.00	6.20
MOTA	2033	CA	LEU			22.836	14.598	-3.085	1.00	18.44
ATOM	2034	CB	LEU	307			15.349	-2.934	1.00	18.44
MOTA	2035	CG	LEU	307		24.157	14.529	-2.083	1.00	18.44
MOTA	2036		LEU	307		25.127		-4.303	1.00	18.44
MOTA	2037		LEU	307		24.744	15.651		1.00	6.20
MOTA	2038	C	LEU	307		20.413	14.550	-3.562		18.44
MOTA	2039	0	LEU	307		19.789	14.910	-2.561	1.00	
MOTA	2040	N	THR	308		19.993	13.589	-4.379	1.00	50.96
MOTA	2041	CA	THR	308		18.753	12.861	-4.133	1.00	50.96
MOTA	2042	CB	THR	308	•	18.299	12.053	-5.389	1.00	9.59
ATOM	2043	OG1	THR	308		19.303	11.094	-5.751	1.00	9.59
ATOM	2044	CG2	THR	308		18.040	12.992	-6.557	1.00	9.59
ATOM	2045	C	THR	308		18.953	11.929	-2.928	1.00	50.96
MOTA	2046	0	THR	308		20.082	11.559	-2.596	1.00	9.59
ATOM	2047	N	PHE	309		17.856	11.538	-2.289	1.00	9.28
ATOM	2048	CA	PHE	309		17.953	10.679	-1.123	1.00	9.28
ATOM	2049	CB	PHE	309		16.612	10.561	-0.421	1.00	35.97
ATOM	2050	CG	PHE	309		16.280	11.795	0.378	1.00	35.97
	2050		PHE	309		16.772	11.950	1.675	1.00	35.97
MOTA				309		15.577	12.854	-0.203	1.00	35.97
ATOM	2052		PHE			16.575	13.149	2.387		35.97
MOTA	2053		PHE	309			14.062	0.497	1.00	35.97
ATOM	2054		PHE	309		15.373		1.796	1.00	35.97
MOTA	2055	CZ	PHE	309		15.875	14.205			9.28
MOTA	2056		PHE	309		18.637	9.355	-1.354		35.97
MOTA	2057		PHE	309		19.450		-0.542		38.48
MOTA	2058		PRO	310		18.371				
ATOM	2059	CD	PRO	310		17.483				23.38
ATOM	2060	CA	PRO	310		19.075				38.48
MOTA	2061	CB	PRO	310		18.467				23.38
ATOM	2062	CG	PRO	310		18.106				23.38
MOTA	2063		PRO	310		20.584	7.675	-2.794	1.00	38.48



## FIG. 3JJ

									22.20
MOTA	2064	0	PRO	310	21.373	6.834	-2.378	1.00	23.38
MOTA	2065	N	LYS	311	20.971	8.846	-3.308	1.00	13.04 13.04
MOTA	2066	CA	LYS	311	22.385	9.214	-3.465	1.00	34.06
MOTA	2067	CB	LYS	311	22.523	10.463	-4.342	1.00	34.06
MOTA	2068	CG	LYS	311	22.808	10.195	-5.807	1.00	34.06
MOTA	2069	CD	LYS	311	24.240	9.693	-6.011	1.00	34.06
MOTA	2070	CE	LYS	311	24.521	9.395	-7.494	1.00	34.06
MOTA	2071	NZ	LYS	311	25.967	9.063	-7.743	1.00 1.00	13.04
ATOM	2072	C	LYS	311	23.019	9.494	-2.105	1.00	34.06
MOTA	2073	0	LYS	311	24.187	9.171	-1.865	1.00	30.77
MOTA	2074	N	LEU	312	22.234	10.137	-1.241	1.00	30.77
MOTA	2075	CA	LEU	312	22.635	10.500	0.118	1.00	12.53
MOTA	2076	CB	LEU	312	21.673	11.556	0.665	1.00	12.53
MOTA	2077	CG	LEU	312	21.900	13.005	0.240	1.00	12.53
MOTA	2078		LEU	312	20.660	13.854	0.540	1.00	12.53
MOTA	2079	CD2	LEU	312	23.134	13.523	0.958	1.00	30.77
ATOM	2080	С	LEU	312	22.658	9.285	1.060	1.00	12.53
MOTA	2081	0	LEU	312	23.514	9.193	1.953	1.00	9.82
MOTA	2082	N	PHE	313	21.709	8.376	0.860 1.668	1.00	9.82
MOTA	2083	CA	PHE	313	21.600	7.167		1.00	19.45
MOTA	2084	CB	PHE	313	20.302	7.155	2.486	1.00	19.45
MOTA	2085	CG	PHE	313	20.168	8.307	3.440 4.522	1.00	19.45
ATOM	2086	CD1	PHE	313	21.030	8.435		1.00	19.45
MOTA	2087	CD2		313	19.182	9.268	3.235		19.45
MOTA	2088	CEl	PHE	313	20.930	9.493	5.385	1.00 1.00	19.45
MOTA	2089	CE2		313	19.056	10.349	4.085		19.45
MOTA	2090	cz	PHE	313	19.938	10.468	5.172	1.00	9.82
ATOM	2091	С	PHE	313	21.559	5.977	0.718	1.00	
MOTA	2092	0	PHE	313	20.501	5.371	0.525	1.00	19.45
MOTA	2093	N	PRO	314	22.709	5.608	0.128	1.00	17.77 21.65
MOTA	2094	CD	PRO	314	24.077	6.031	0.454	1.00	17.77
MOTA	2095	CA	PRO	314	22.726	4.474	-0.797	1.00	21.65
MOTA	2096	CB	PRO	314	24.203	4.367	-1.168	1.00	21.65
MOTA	2097	CG	PRO	314	24.881	4.791	0.098	1.00	17.77
ATOM	2098	C	PRO	314	22.227	3.213	-0.114	1.00	21.65
ATOM	2099	0	PRO	314	22.160	3.142	1.111	1.00	38.72
MOTA	2100	N	ASP	315	21.889	2.215	-0.919	1.00	38.72
MOTA	2101	CA	ASP	315	21.380	0.941	-0.422	1.00	47.92
MOTA	2102	CB	ASP	315	21.078	0.026	-1.610	1.00	47.92
ATOM	2103	CG	ASP	315	20.157	0.687	-2.626	1.00	47.92
ATOM	2104		L ASP	315	18.939	0.386	-2.604	1.00	47.92
MOTA	2105	OD2	2 ASP	315	20.646	1.517	-3.434	1.00	38.72
MOTA	2106	C	ASP	315	22.324	0.248	0.568	1.00	47.92
MOTA	2107	0	ASP	315	21.888	-0.275	1.600	1.00	22.14
ATOM	2108	N	SER	316	23.623		0.301	1.00	22.14
ATOM	2109	CA	SER	316	24.645		1.130		
MOTA	2110	CB	SER	316	26.022				41.15 41.15
MOTA	2111	OG	SER	316	26.118				22.14
MOTA	2112	C	SER	316	24.587				
ATOM	2113	0	SER	316	25.207				41.15
MOTA	2114	N	LEU	317	23.846				35.08
ATOM	2115	CA	LEU	317	23.741				35.08
ATOM	2116	CB	LEU	317	23.445				17.46
ATOM	2117		<b>LEU</b>	317	24.520				17.46
MOTA	2118		1 LEU	317	24.047				17.46
MOTA	2119	CD	2 LEU	317	25.812				17.46
MOTA	2120		LEU	317	22.659				35.08
MOTA	2121	. 0	LEU	317	22.862				17.46
MOTA	2122	N	PHE	318	21.531	0.455	4.435	1.00	4.02



## FIG. 3KK

ATOM	2123	CA	PHE	318	20.392	-0.278	4.954	1.00	4.02
MOTA	2124	CB	PHE	318	19.113	0.147	4.230	1.00	16.56
ATOM	2125	CG	PHE	318	18.903	1.640	4.201	1.00	16.56
MOTA	2126	CD1	PHE	318	18.133	2.268	5.174	1.00	16.56
ATOM	2127	CD2	PHE	318	19.514	2.420	3.216	1.00	16.56
ATOM	2128	CE1		318	17.977	3.655	5.175	1.00	16.56
ATOM	2129	CE2	PHE	318	19.373	3.805	3.201	1.00	16.56
ATOM	2130	CZ	PHE	318	18.602	4.430	4.182	1.00	16.56
ATOM	2131	C	PHE	318	20.591	-1.758	4.744	1.00	4.02
ATOM	2132	Ō	PHE	318	21.200	-2.172	3.761	1.00	16.56
ATOM	2133	N	PRO	319	20.151	-2.578	5.708	1.00	31.17
MOTA	2134	CD	PRO	319	19.637	-2.218	7.040	1.00	52.46
ATOM	2135	CA	PRO	319	20.289	-4.029	5.574	1.00	31.17
ATOM	2136	CB	PRO	319	19.834	-4.543	6.951	1.00	52.46
ATOM	2137	CG	PRO	319	18.905	-3.478	7.455	1.00	52.46
ATOM	2138	C	PRO	319	19.339	-4.452	4.451	1.00	31.17
	2139	0	PRO	319	18.128	-4.225	4.536	1.00	52.46
ATOM	2140	N	ALA	320	19.881	-5.025	3.384	1.00	10.87
ATOM		CA	ALA	320	19.059	-5.424	2.257	1.00	10.87
MOTA	2141 2142	CB	ALA	320	19.248	-4.435	1.107	1.00	25.21
MOTA		C	ALA	320	19.414	-6.826	1.808	1.00	10.87
ATOM	2143		ALA	320	19.881	-7.020	0.685	1.00	25.21
MOTA	2144	0	ASP	321	19.203	-7.804	2.685	1.00	47.66
MOTA	2145	N		321	19.521	-9.181	2.338	1.00	47.66
MOTA	2146	CA	ASP ASP		20.236	-9.900	3.483	1.00	64.42
MOTA	2147	CB		321 321		-11.050	2.986	1.00	64.42
ATOM	2148	CG	ASP			-11.200	1.744	1.00	64.42
MOTA	2149		ASP	321		-11.811	3.820	1.00	64.42
MOTA	2150		ASP	321	18.294	-9.956	1.891	1.00	47.66
ATOM	2151	C	ASP	321		-10.675	0.893	1.00	64.42
MOTA	2152	0	ASP	321	17.222	-9.840	2.661	1.00	3.49
MOTA	2153	Ŋ	SER	322		-10.494	2.337	1.00	3.49
MOTA	2154	CA	SER	322		-10.922	3.612	1.00	13.00
MOTA	2155	CB	SER	322		-9.836	4.520	1.00	13.00
MOTA	2156	OG	SER	322	15.170	-9.500	1.589	1.00	3.49
MOTA	2157	C	SER	322	15.094	-8.315	1.528	1.00	13.00
MOTA	2158	0	SER	322	15.394	-9.983	1.070	1.00	2.00
MOTA	2159	N	GLU	323	13.978	-9.146	0.331	1.00	2.00
ATOM	2160	CA	GLU	323	13.051	-10.007	-0.567	1.00	23.86
MOTA	2161	CB	GLU	323			-1.886	1.00	23.86
MOTA	2162	CG	GLU	323	11.838	-9.356	-3.036	1.00	23.86
ATOM	2163	CD	GLU	323	12.668	-9.902	-3.713	1.00	23.86
MOTA	2164		L GLU	323		-10.834	-3.713	1.00	23.86
MOTA	2165		2 GLU	323	13.781	-9.396	1.276	1.00	2.00
MOTA	2166	C	GLU	323	12.194		0.837	1.00	23.86
MOTA	2167	0	GLU	323	11.431			1.00	17.95
MOTA	2168	N	HIS	324	12.283		2.570 3.605	1.00	17.95
MOTA	2169	CA	HIS	324	11.560		4.834	1.00	5.49
MOTA	2170	CB	HIS	324	11.312			1.00	5.49
MOTA	2171	CG		324	10.841		6.060	1.00	5.49
MOTA	2172		2 HIS	324	9.611		6.596	1.00	5.49
ATOM	2173		1 HIS	324	11.713		6.917	1.00	5.49
MOTA	2174		1 HIS	324	11.036		7.928	1.00	5.49
MOTA	2175		2 HIS	324	9.759		7.763		17.95
MOTA	2176	С	HIS	324	12.466		3.969		5.49
MOTA	2177	0	HIS	324	12.003		4.224		
MOTA	2178	N	ASN	325	13.767		3.993		2.00
ATOM	2179			325	14.774		4.293		2.00 16.84
MOTA	2180	CB	ASN	325	16.103	-6.609	4.656	1.00	10.04

FIG. 3LL

ATOM	2181	CG	ASN	325	16.090	-7.208	6.039	1.00	16.84
ATOM	2182	OD1	ASN	325	15.032	-7.379	6.645	1.00	16.84
ATOM	2183	ND2	ASN	325	17.263	-7.517	6.558	1.00	16.84
ATOM	2184	C	ASN	325	14.984	-5.004	3.122	1.00	2.00
ATOM	2185	0	ASN	325	15.645	-3.982	3.246	1.00	16.84
MOTA	2186	N	LYS	326	14.468	-5.386	1.964	1.00	23.08
ATOM	2187	CA	LYS	326	14.582	-4.552	0.791	1.00	23.08
ATOM	2188	CB	LYS	326	14.644	-5.405	-0.475	1.00	28.36
ATOM	2189	CG	LYS	326	15.917	-6.240	-0.575	1.00	28.36
ATOM	2190	CD	LYS	326	15.960	-6.997	-1.888	1.00	28.36
ATOM	2191	CE	LYS	326	17.085	-8.035	-1.946	1.00	28.36
ATOM	2192	NZ	LYS	326	18.456	-7.449	-2.017	1.00	28.36
ATOM	2193	С	LYS	326	13.387	-3.608	0.766	1.00	23.08
ATOM	2194	0	LYS	326	13.531	-2.426	0.465	1.00	28.36
MOTA	2195	N	LEU	327	12.220	-4.107	1.150	1.00	2.00
ATOM	2196	CA	LEU	327	11.028	-3.277	1.165	1.00	2.00
MOTA	2197	CB	LEU	327	9.772	-4.119	1.385	1.00	8.67
MOTA	2198	CG	LEU	327	8.421	-3.402	1.491	1.00	8.67
ATOM	2199	CD1	LEU	327	8.096	-2.695	0.196	1.00	8.67
ATOM	2200	CD2	LEU	327	7.319	-4.379	1.836	1.00	8.67
ATOM	2201	С	LEU	327	11.150	-2.229	2.249	1.00	2.00
ATOM	2202	0	LEU	327	10.984	-1.047	1.993	1.00	8.67
ATOM	2203	N	LYS	328	11.489	-2.656	3.452	1.00	2.57
ATOM	2204	CA	LYS	328	11.634	-1.739	4.570	1.00	2.57
MOTA	2205	СВ	LYS	328	11.946	-2.510	5.852	1.00	9.10
MOTA	2206	CG	LYS	328	10.761	-3.238	6.441	1.00	9.10
MOTA	2207	CD	LYS	328	9.688	-2.273	6.894	1.00	9.10
MOTA	2208	CE	LYS	328	8.459	-3.009	7.391	1.00	9.10
MOTA	2209	NZ	LYS	328	7.431	-2.129	8.011	1.00	9.10
MOTA	2210	C	LYS	328	12.703	-0.680	4.324	1.00	2.57
MOTA	2211	0	LYS	328	12.585	0.441	4.802	1.00	9.10
MOTA	2212	N	ALA	329	13.716	-1.029	3.541	1.00	13.58
MOTA	2213	CA	ALA	329	14.804	-0.117	3.230	1.00	13.58
MOTA	2214	CB	ALA	329	15.970	-0.865	2.596	1.00	16.18
ATOM	2215	C	ALA	329	14.337	0.997	2.317	1.00	13.58
MOTA	2216	0	ALA	329	14.899	2.079	2.341	1.00	16.18
MOTA	2217	N	SER	330	13.330	0.726	1.491	1.00	11.09
MOTA	2218	CA	SER	330	12.785	1.737	0.593	1.00	11.09
MOTA	2219	CB	SER	330	12.081	1.100	-0.611	1.00	11.72
MOTA	2220	OG	SER	330	10.754	0.706	-0.292	1.00	11.72
MOTA	2221	С	SER	330	11.806	2.581	1.404	1.00	11.09
MOTA	2222	0	SER	330	11.557	3.743	1.093	1.00	11.72
MOTA	2223	N	GLN	331	11.266	1.986	2.461	1.00	2.00
MOTA	2224	CA	GLN	331	10.333	2.679	3.335	1.00	6.13
MOTA	2225	CB	GLN	331	9.517	1.664	4.131	1.00	6.13
MOTA	2226	CG	GLN	331	8.571	0.855	3.293		6.13
MOTA	2227	CD	GLN	331	7.766	-0.121	4.097		6.13
MOTA	2228		GLN	331	8.024	-0.337	5.265	1.00	6.13
ATOM	2229		GFM	331	6.795	-0.740	3.463		2.00
MOTA	2230	C	GLN	331	11.058	3.617	4.298		6.13
ATOM	2231	0	GLN	331	10.513	4.639	4.717		5.63
ATOM	2232	N	ALA		12.277	3.235	4.660	1.00	5.63
MOTA	2233	CA	ALA		13.102	3.992	5.583	1.00	19.90
MOTA	2234	CB	ALA		14.277	3.151	6.043	1.00	5.63
ATOM	2235	C	ALA		13.603	5.241	4.909		19.90
ATOM	2236	0	ALA		13.528	6.333	5.459		2.00
ATOM	2237	N	ARG		14.053	5.080	3.676		2.00
MOTA	2238	CA	ARG	333	14.575	6.186	2.902	1.00	2.00

### FIG. 3MM

ATOM	2239	СВ	ARG	333	15.351	5.665	1.703	1.00	16.50
ATOM	2240	CG	ARG	333	16.331	6.648	1.131	1.00	16.50
MOTA	2241	CD	ARG	333	16.800	6.190	-0.246	1.00	16.50
MOTA	2242	NE	ARG	333	17.762	5.090	-0.231	1.00	16.50
MOTA	2243	CZ	ARG	333	17.581	3.920	-0.842	1.00	16.50
MOTA	2244	NH1	ARG	333	16.452	3.680	-1.502	1.00	16.50
MOTA	2245	NH2	ARG	333	18.572	3.028	-0.877	1.00	16.50
MOTA	2246	C	ARG	333	13.442	7.095	2.461	1.00	2.00
MOTA	2247	0	ARG	333	13.655	8.281	2.266	1.00	16.50
MOTA	2248	N	ASP	334	12.229	6.561	2.349	1.00	2.00
MOTA	2249	CA	ASP	334	11.095	7.377	1.953	1.00	2.00 11.10
MOTA	2250	CB	ASP	334	9.887	6.522	1.588	1.00	
MOTA	2251	CG	ASP	334	8.753	7.341	0.973	1.00	11.10
MOTA	2252		ASP	334	8.940	7.907	-0.137	1.00	11.10
MOTA	2253		ASP	334	7.670	7.412	1.594	1.00	11.10
MOTA	2254	С	ASP	334	10.712	8.286	3.110	1.00	2.00
MOTA	2255	0	ASP	334	10.309	9.425	2.904	1.00	11.10 2.00
ATOM	2256	N	LEU	335	10.803	7.756	4.325	1.00	
MOTA	2257	CA	LEU	335	10.486	8.491	5.536	1.00	2.00 2.00
MOTA	2258	CB	LEU	335	10.486	7.523	6.717	1.00	
MOTA	2259	CG	LEU	335	10.094	7.963	8.118	1.00	2.00
MOTA	2260		PEA	335	8.660	8.436	8.151	1.00	2.00 2.00
MOTA	2261		LEU	335	10.295	6.800	9.052	1.00	2.00
MOTA	2262	С	LEU	335	11.555	9.561	5.700	1.00	2.00
MOTA	2263	0	LEU	335	11.239	10.719	5.931	1.00	2.00
MOTA	2264	N	LEU	336	12.814	9.181	5.511	1.00	2.14
MOTA	2265	CA	LEU	336	13.925	10.111	5.611	1.00	8.04
MOTA	2266	CB	LEU	336	15.250	9.392	5.335	1.00	8.04
ATOM	2267	CG	LEU	336	16.116	8.862	6.472 5.941	1.00 1.00	8.04
ATOM	2268		LEU	336	17.147	7.889	7.172	1.00	8.04
MOTA	2269		LEU	336	16.786	10.022 11.280	4.625	1.00	2.14
MOTA	2270	C	LEU	336	13.775	12.423	4.968	1.00	8.04
MOTA	2271	0	LEU	336	14.096	10.995	3.419	1.00	2.00
ATOM	2272	N	SER	337	13.277	12.009	2.386	1.00	2.00
ATOM	2273	CA	SER	337	13.098	11.367	1.024	1.00	2.98
ATOM	2274	CB	SER	337	12.788	10.693	1.024	1.00	2.98
MOTA	2275	OG	SER	337	11.543	13.024	2.722	1.00	2.00
MOTA	2276	C	SER	337	12.022 11.999	14.103	2.151	1.00	2.98
ATOM	2277	0	SER	337	11.110	12.658	3.616	1.00	3.30
ATOM	2278	N	LYS	338 338	10.031	13.539	4.030	1.00	3.30
MOTA	2279	CA	LYS	338	8.796	12.733	4.438	1.00	10.86
ATOM	2280	CB CG	LYS LYS	338	8.340	11.631	3.484	1.00	10.86
MOTA	2281 2282	CD	LYS	338	7.473	12.142	2.349	1.00	10.86
ATOM	2282	CE	LYS	338	6.938	10.996	1.524	1.00	10.86
ATOM	2283	NZ	LYS	338	6.052	10.123	2.334	1.00	10.86
MOTA	2284	C	LYS	338	10.488	14.372	5.225	1.00	3.30
ATOM	2286	0	LYS	338	10.169	15.553	5.329	1.00	10.86
ATOM	2287	N	MET	339	11.242	13.752	6.123	1.00	2.00
MOTA	2288	CA	MET	339	11.725	14.425	7.316	1.00	2.00
ATOM ATOM	2289	CB	MET	339	12.139	13.396	8.375	1.00	2.00
ATOM	2290	CG	MET	339	10.999	12.536	8.901	1.00	2.00
	2291	SD	MET	339	11.504	11.362	10.161	1.00	2.00
ATOM ATOM	2291	CE	MET	339	10.004	11.147	10.942	1.00	2.00
MOTA	2293	CE	MET	339	12.868	15.396	7.064	1.00	2.00
ATOM	2294	0	MET	339	12.906	16.483	7.638	1.00	2.00
ATOM	2295	N	LEU		13.806	15.012	6.213	1.00	2.00
ATOM	2296	CA			14.915	15.894	5.930	1.00	2.00
ATOM	2297	CB	LEU		16.172	15.110	5.603	1.00	7.41
ATOM	4431	CD	11EU	240	10.172		2.000		



## FIG. 3NN

									- 43
MOTA	2298	CG	LEU	340	16.789	14.652	6.915	1.00	7.41
ATOM	2299	CD1		340	18.085	13.954	6.639	1.00	7.41
MOTA	2300	CD2	LEU	340	17.013	15.839	7.837	1.00	7.41
ATOM	2301	C	LEU	340	14.600	16.919	4.867	1.00	2.00
MOTA	2302	0	LEU	340	15.307	17.051	3.882	1.00	7.41
MOTA	2303	N	VAL	341	13.535	17.668	5.111	1.00	12.82
MOTA	2304	CA	VAL	341	13.080	18.721	4.226	1.00	12.82
ATOM	2305	CB	VAL	341	11.574	18.576	3.963	1.00	9.51
ATOM	2306	CG1	VAL	341	11.089	19.709	3.100	1.00	9.51
ATOM	2307	CG2	VAL	341	11.294	17.253	3.300	1.00	9.51
ATOM	2308	C	VAL	341	13.383	20.063	4.914	1.00	12.82
ATOM	2309	Ō	VAL	341	13.079	20.238	6.093	1.00	9.51
ATOM	2310	N	ILE	342	14.000	20.996	4.190	1.00	4.21
ATOM	2311	CA	ILE	342	14.364	22.298	4.748	1.00	4.21
ATOM	2312	CB	ILE	342	15.462	22.984	3.900	1.00	6.31
ATOM	2313	CG2		342	15.799	24.360	4.452	1.00	6.31
ATOM	2314		ILE	342	16.719	22.108	3.900	1.00	6.31
ATOM	2315	CD1		342	17.843	22.656	3.067	1.00	6.31
MOTA	2316	C	ILE	342	13.182	23.224	4.975	1.00	4.21
ATOM	2317	Ö	ILE	342	13.117	23.883	6.016	1.00	6.31
ATOM	2317	N	ASP	343	12.236	23.255	4.041	1.00	2.00
	2319	CA	ASP	343	11.065	24.108	4.191	1.00	2.00
MOTA	2320	CB	ASP	343	10.494	24.501	2.823	1.00	21.74
ATOM	2321	CG	ASP	343	9.258	25.414	2.926	1.00	21.74
MOTA			ASP	343	9.113	26.183	3.915	1.00	21.74
MOTA	2322 2323		ASP	343	8.421	25.366	1.998	1.00	21.74
MOTA		C	ASP	343	10.009	23.390	5.026	1.00	2.00
ATOM	2324		ASP	343	9.532	22.328	4.654	1.00	21.74
ATOM	2325	0	PRO	344	9.661	23.949	6.191	1.00	12.51
MOTA	2326	N		344	10.281	25.161	6.751	1.00	16.37
MOTA	2327	CD	PRO	344	8.660	23.408	7.120	1.00	12.51
MOTA	2328	CA	PRO PRO	344	8.633	24.449	8.234	1.00	16.37
MOTA	2329	CB			9.997	25.012	8.214	1.00	16.37
MOTA	2330	CG	PRO	344	7.269	23.236	6.516	1.00	12.51
ATOM	2331	C	PRO	344	6.469	22.473	7.040	1.00	16.37
MOTA	2332	0	PRO	344	6.960	23.979	5.455	1.00	11.95
MOTA	2333	N	ALA	345	5.657	23.872	4.816	1.00	11.95
ATOM	2334	CA	ALA	345	5.416	25.044	3.881	1.00	9.14
ATOM	2335	CB	ALA	345	5.515	22.558	4.070	1.00	11.95
ATOM	2336	C	ALA	345	4.420	22.018	3.967	1.00	9.14
ATOM	2337	0	ALA	345	6.634	22.016	3.580	1.00	2.00
ATOM	2338	И	LYS	346	6.655	20.776	2.840	1.00	2.00
MOTA	2339	CA	LYS	346	7.534	20.770	1.595	1.00	15.05
MOTA	2340	CB	LYS	346	6.984	21.930	0.601	1.00	15.05
ATOM	2341	CG	LYS	346		22.442	-0.340	1.00	15.05
ATOM	2342	CD	LYS	346	8.067	23.576	-1.222	1.00	15.05
MOTA	2343	CE	LYS	346	7.529	23.576	-0.427	1.00	15.05
MOTA	2344	NZ	LYS	346	7.093	19.597	3.695	1.00	2.00
ATOM	2345	C	LYS	346	7.131	18.442	3.279	1.00	15.05
MOTA	2346	0	LYS	346	7.046		4.903	1.00	2.00
ATOM	2347	N	ARG	347	7.602	19.900	5.828	1.00	2.00
MOTA	2348	CA		347	8.081	18.881	6.939	1.00	3.45
MOTA	2349	CB	ARG	347	8.913	19.498	7.598	1.00	3.45
MOTA	2350	CG		347	9.801	18.490	8.775		3.45
ATOM	2351	CD		347	10.512	19.071	8.775		3.45
MOTA	2352	NE		347	11.486		8.893		3.45
MOTA	2353	CZ		347	11.548		9.833	1.00	3.45
MOTA	2354		1 ARG	347	10.686				3.45
ATOM	2355		2 ARG	347	12.452		8.450		2.00
MOTA	2356	C	ARG	347	6.906	18.134	6.431	1.00	2.00



FIG. 300

MOTA	2357	0	ARG	347	5.832	18.694	6.614	1.00	3.45
ATOM	2358	N	ILE	348	7.120	16.860	6.732	1.00	2.29
ATOM	2359	CA	ILE	348	6.088	15.991	7.288	1.00	2.29
MOTA	2360	CB	ILE	348	6.431	14.489	7.057	1.00	2.00
ATOM	2361	CG2	ILE	348	7.530	14.026	8.012	1.00	2.00
ATOM	2362	CG1	ILE	348	5.174	13.639	7.234	1.00	2.00
MOTA	2363	CD1	ILE	348	5.351	12.213	6.784	1.00	2.00
ATOM	2364	C	ILE	348	5.821	16.240	8.758	1.00	√2.29
ATOM	2365	ō	ILE	348	6.733	16.518	9.532	1.00	2.00
ATOM	2366	N	SER	349	4.550	16.127	9.127	1.00	5.28
MOTA	2367	CA	SER	349	4.106	16.351	10.494	1.00	5.28
ATOM	2368	CB	SER	349	2.612	16.722	10.515	1.00	14.72
MOTA	2369	OG	SER	349	1.814	15.800	9.786	1.00	14.72
ATOM	2370	C	SER	349	4.357	15.122	11.350	1.00	5.28
	2370	0	SER	349	4.721	14.067	10.839	1.00	14.72
MOTA		N	VAL	350	4.146	15.251	12.653	1.00	20.79
MOTA	2372		VAL	350	4.357	14.140	13.561	1.00	20.79
ATOM	2373	CA	VAL	350	4.321	14.594	15.044	1.00	18.92
ATOM	2374	CB			4.677	13.434	15.953	1.00	18.92
MOTA	2375		VAL	350	5.296	15.740	15.269	1.00	18.92
MOTA	2376		VAL	350	3.296	13.740	13.325	1.00	20.79
MOTA	2377	C	VAL	350	3.606	11.883	13.340	1.00	18.92
MOTA	2378	0	VAL	350		13.495	13.055	1.00	2.00
MOTA	2379	N	ASP	351	2.063	12.568	12.827	1.00	2.00
MOTA	2380	CA	ASP	351	0.953		12.900	1.00	23.45
ATOM	2381	CB	ASP	351	-0.371	13.321	14.234	1.00	23.45
MOTA	2382	CG	ASP	351	-0.559	14.012	14.234	1.00	23.45
MOTA	2383		ASP	351	-0.281	15.234		1.00	23.45
MOTA	2384		ASP	351	-0.945	13.316	15.198	1.00	2.00
MOTA	2385	C	ASP	351	1.024	11.760	11.545	1.00	23.45
MOTA	2386	0	ASP	351	0.484	10.661	11.468		17.97
MOTA	2387	N	ASP	352	1.674	12.315	10.531	1.00	17.97
MOTA	2388	CA	ASP	352	1.829	11.616	9.263	1.00	2.54
ATOM	2389	CB	ASP	352	1.957	12.598	8.108	1.00	
MOTA	2390	CG	ASP	352	0.642	13.267	7.759	1.00	2.54
ATOM	2391		ASP	352	-0.436	12.730	8.135	1.00	2.54
MOTA	2392	OD2	ASP	352	0.695	14.329	7.118	1.00	2.54
ATOM	2393	С	ASP	352	3.024	10.699	9.314	1.00	17.97
MOTA	2394	0	ASP	352	3.035	9.667	8.648	1.00	2.54
MOTA	2395	N	ALA	353	4.011	11.064	10.129	1.00	2.00
ATOM	2396	CA	ALA	353	5.224	10.270	10.310	1.00	2.00
MOTA	2397	CB	ALA	353	6.289	11.079	11.024	1.00	13.93
MOTA	2398	С	ALA	353	4.884	9.014	11.107	1.00	2.00
MOTA	2399	0	ALA	353	5.600	8.024	11.044	1.00	13.93
ATOM	2400	N	LEU	354	3.769	9.063	11.831	1.00	2.00
MOTA	2401	CA	LEU	354	3.300	7.942	12.629	1.00	2.00
ATOM	2402	CB	LEU	354	2.517	8.458	13.827	1.00	10.71
MOTA	2403	CG	LEU	354	3.359	9.011	14.967	1.00	10.71
ATOM	2404		l LEU	354	2.548	10.017	15.749	1.00	10.71
MOTA	2405		2 LEU	354	3.860	7.875	15.853	1.00	10.71
ATOM	2406		LEU	354	2.431	7.001	11.811	1.00	2.00
ATOM	2407		LEU	354	2.219	5.854	12.198		10.71
ATOM	2408		GLN	355	1.889	7.517	10.709	1.00	2.00
ATOM	2409			355	1.049		9.806	1.00	2.00
ATOM	2410			355	-0.143			1.00	23.61
ATOM	2411			355	-1.341			1.00	23.61
ATOM	2412			355	-1.835				23.61
MOTA	2413		1 GLN	355	-2.113				23.61
ATOM	2414		2 GLN	355	-1.951			1.00	23.61
ATOM	2415		GLN	355	1.854				2.00
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FIG. 3PP

									1 00	22 61
MOTA	2416	0	GLN	355		1.308	5.669	7.686	1.00	23.61 2.14
ATOM	2417	N	HIS	356		3.157	6.505	8.651	1.00	2.14
MOTA	2418	CA	HIS	356		4.042	6.074	7.584	1.00	10.92
ATOM	2419	CB	HIS	356		5.407	6.747	7.735		10.92
MOTA	2420	CG	HIS	356		6.262	6.667	6.510	1.00	10.92
MOTA	2421		HIS	356		7.183	5.756	6.117	1.00	10.92
ATOM	2422	ND1	HIS	356		6.227	7.626	5.523	1.00	
MOTA	2423	CE1	HIS	356		7.094	7.311	4.577	1.00	10.92
MOTA	2424	NE2	HIS	356		7.686	6.180	4.915	1.00	10.92
MOTA	2425	C	HIS	356		4.186	4.553	7.711	1.00	2.14
MOTA	2426	0	HIS	356		4.341	4.040	8.808	1.00	10.92
ATOM	2427	N	PRO	357		4.132	3.818	6.590	1.00	13.41
MOTA	2428	CD	PRO	357		3.937	4.297	5.213	1.00	36.38
MOTA	2429	CA	PRO	357		4.262	2.356	6.619	1.00	13.41
MOTA	2430	CB	PRO	357		4.321	1.981	5.134	1.00	36.38
MOTA	2431	CG	PRO	357		4.691	3.289	4.432	1.00	36.38
MOTA	2432	C	PRO	357		5.476	1.836	7.397	1.00	13.41
MOTA	2433	0	PRO	357		5.395	0.788	8.043	1.00	36.38
ATOM	2434	N	TYR	358		6.590	2.563	7.371	1.00	5.90 5.90
MOTA	2435	CA	TYR	358		7.765	2.113	8.098	1.00	
MOTA	2436	CB	TYR	358		8.996	2.933	7.709	1.00	6.75
MOTA	2437	CG	TYR	358		10.315	2.361	8.174	1.00	6.75
MOTA	2438	CD1	TYR	358		10.694	1.069	7.851	1.00	6.75
MOTA	2439		TYR	358		11.943	0.571	8.214	1.00	6.75 6.75
MOTA	2440	CD2	TYR	358		11.218	3.143	8.877	1.00	6.75
ATOM	2441	CE2	TYR	358		12.465	2.653	9.245	1.00	6.75
MOTA	2442	CZ	TYR	358	•	12.826	1.369	8.905	1.00	6.75
MOTA	2443	OH	TYR	358		14.074	0.902	9.247	1.00 1.00	5.90
MOTA	2444	C	TYR	358		7.503	2.210	9.604	1.00	6.75
ATOM	2445	0	TYR	358		8.002	1.385	10.356	1.00	20.57
MOTA	2446	N	ILE	359		6.672	3.169	11.457	1.00	20.57
MOTA	2447	CA	ILE	359		6.357	3.387 4.917	11.829	1.00	2.00
MOTA	2448	CB	ILE	359		6.402	5.121	13.318	1.00	2.00
MOTA	2449	CG2		359		6.153 7.754	5.527	11.478	1.00	2.00
MOTA	2450	CGI		359		8.870	5.038	12.334	1.00	2.00
ATOM	2451		LILE	359 359		5.022	2.835	11.996	1.00	20.57
ATOM	2452	C	ILE	359		4.980	2.229	13.070	1.00	2.00
ATOM	2453	0	ASN	360		3.943	3.040	11.249	1.00	11.50
MOTA	2454 2455	N CA	ASN	360		2.600	2.617	11.647	1.00	11.50
MOTA	2455 2456	CB	ASN	360		1.587	2.863	10.519	1.00	15.91
MOTA MOTA	2450		ASN	360		1.535	1.720	9.513	1.00	15.91
	2458		1 ASN	360		2.554	1.310	8.974	1.00	15.91
MOTA MOTA	2459		2 ASN	360		0.338	1.198	9.270	1.00	15.91
ATOM	2460		ASN	360		2.490	1.170	12.110	1.00	11.50
MOTA	2461		ASN	360		1.581	0.836	12.871	1.00	15.91
MOTA	2462		VAL	361		3.415	0.318	11.670	1.00	2.00
MOTA	2463			361		3.374	-1.083	12.050	1.00	2.00
ATOM	2464			361		4.517	-1.914	11.398	1.00	43.19
ATOM	2465		1 VAL	361		4.397	-1.886	9.872		43.19
MOTA	2466		2 VAL	361		5.885	-1.429	11.860		43.19
ATOM	2467		VAL	361		3.400	-1.280	13.565		2.00
MOTA	2468		VAL	361		3.067	-2.357	14.051		43.19
ATOM	2469		TRP	362		3.742	-0.234	14.311		2.00
MOTA	2470			362		3.794	-0.325	15.766		2.00
MOTA	2471		TRP	362		5.143	0.178	16.285		4.01
ATOM	2472			362		6.316	-0.475	15.704		4.01
MOTA	2473	CI	2 TRP	362		6.938	-1.674	16.168		4.01
MOTA	2474	E CE	2 TRP	362		8.076	-1.890	15.371	1.00	4.01



FIG. 3QQ

ATOM	2475	CE3	TRP	362	6.643	-2.580	17.189	1.00	4.01
ATOM	2476	CD1		362	7.074	-0.028	14.666	1.00	4.01
ATOM	2477	NE1	TRP	362	8.135	-0.872	14.459	1.00	4.01
ATOM	2478	CZ2	TRP	362	8.928	-2.987	15.566	1.00	4.01
ATOM	2479	CZ3	TRP	362	7.482	-3.662	17.383	1.00	4.01
ATOM	2480	CH2	TRP	362	8.614	-3.857	16.578	1.00	4.01
MOTA	2481	C	TRP	362	2.716	0.497	16.454	1.00	2.00
ATOM	2482	0	TRP	362	2.496	0.329	17.641	1.00	4.01
ATOM	2483	N	TYR	363	2.039	1.362	15.706	1.00	9.42
ATOM	2484	CA	TYR	363	1.013	2.268	16.228	1.00	9.42
ATOM	2485	CB	TYR	363	0.181	2.843	15.073	1.00	9.22
MOTA	2486	CG	TYR	363	-0.775	3.962	15.439	1.00	9.22
MOTA	2487	CD1	TYR	363	-2.064	3.688	15.899	1.00	9.22
ATOM	2488	CE1	TYR	363	-2.966	4.716	16.182	1.00	9.22
MOTA	2489	CD2	TYR	363	-0.409	5.296	15.278	1.00	9.22
MOTA	2490	CE2	TYR	363	-1.300	6.331	15.568	1.00	9.22
MOTA	2491	CZ	TYR	363	-2.577	6.031	16.016	1.00	9.22
MOTA	2492	OH	TYR	363	-3.485	7.023	16.296	1.00	9.22
MOTA	2493	C	TYR	363	0.091	1.694	17.301	1.00	9.42
MOTA	2494	0	TYR	363	-0.451	0.590	17.150	1.00	9.22
ATOM	2495	N	ASP	364	-0.073	2.461	18.381	1.00	23.57
MOTA	2496	CA	ASP	364	-0.923	2.100	19.516	1.00	23.57 8.62
MOTA	2497	CB	ASP	364	-0.078	1.494	20.651	1.00	8.62
MOTA	2498	CG	ASP	364	-0.916	0.800	21.737	1.00	8.62
MOTA	2499		ASP	364	-2.053	1.246	22.034	1.00	8.62
MOTA	2500	OD2	ASP	364	-0.420	-0.191	22.309	1.00	23.57
MOTA	2501	C	ASP	364	-1.579	3.399	19.971	1.00	8.62
MOTA	2502	0	ASP	364	-0.894	4.376	20.268	1.00	26.34
MOTA	2503	N	PRO	365	-2.918	3.433	20.004	1.00 1.00	36.54
MOTA	2504	CD	PRO	365	-3.819	2.313	19.698	1.00	26.34
MOTA	2505	CA	PRO	365	-3.676	4.616	20.429	1.00	36.54
MOTA	2506	CB	PRO	365	-5.117	4.102	20.455 19.417	1.00	36.54
MOTA	2507	CG	PRO	365	-5.117	3.016	21.824	1.00	26.34
MOTA	2508	C	PRO	365	-3.252	5.043 6.224	22.099	1.00	36.54
MOTA	2509	0	PRO	365	-3.057	4.049	22.691	1.00	34.81
MOTA	2510	N	ALA	366	-3.084	4.273	24.067	1.00	34.81
MOTA	2511	CA	ALA	366	-2.691	2.952	24.811	1.00	23.80
MOTA	2512	CB	ALA	366	-2.627 -1.357	4.979	24.143	1.00	34.81
ATOM	2513	C	ALA	366	-1.198	5.915	24.924	1.00	23.80
ATOM	2514	0	ALA	366	-0.418	4.577	23.292	1.00	15.56
ATOM	2515	N	GLU	367	0.911	5.181	23.301	1.00	15.56
ATOM	2516	CA	GLU	367	1.942	4.223	22.707	1.00	54.26
MOTA	2517	CB	GLU	367 367	2.018	2.895			54.26
ATOM	2518	CG	GLU	367 367	2.873	1.832	22.736	1.00	54.26
MOTA	2519		GLU	367	3.056		21.492		54.26
MOTA	2520		L GLU	367	3.357		23.431		54.26
ATOM	2521		GLU GLU	367	0.941				15.56
ATOM	2522			367	1.694				54.26
MOTA	2523		GLU VAL	368	0.080				52.58
ATOM	2524			368	0.056				52.58
MOTA	2525			368	-0.258				22.16
MOTA	2526		VAL 1 VAL	368	-0.404				22.16
MOTA	2527		2 VAL	368	0.850				22.16
MOTA	2528		VAL VAL	368	-0.931				52.58
MOTA	2529		VAL	368	-0.549				22.16
MOTA	2530 2531		GLU	369	-2.206				23.43
MOTA	2532			369	-3.300				23.43
MOTA	2532			369	-4.561				53.35
MOTA	<u> </u>	می ره	GTO	203	JUI				



## FIG. 3RR

MOTA	2534	CG	GLU	369	-4.450	9.125	19.182	1.00	53.35 53.35
MOTA	2535	CD	GLU	369	-4.518	10.581	18.692	1.00	53.35
MOTA	2536	OE1	GLU	369	-4.879	11.498	19.474 17.503	1.00	53.35
MOTA	2537	OE2	GLU	369	-4.208	10.816 9.381	22.987	1.00	23.43
MOTA	2538	C	GLU	369	-3.566	9.155	23.424	1.00	53.35
MOTA	2539	0	GLU	369	-4.699	9.615	23.770	1.00	27.26
MOTA	2540	N	ALA	370	-2.516	9.660	25.228	1.00	27.26
MOTA	2541	CA	ALA	370	-2.618	9.371	25.858	1.00	10.16
MOTA	2542	CB	ALA	370	-1.253 -3.123	11.050	25.640	1.00	27.26
MOTA	2543	С	ALA	370 370	-2.923	12.021	24.912	1.00	10.16
ATOM	2544	0	ALA	370 371	-3.773	11.159	26.824	1.00	34.01
MOTA	2545	N	PRO PRO	371	-3.949	10.062	27.792	1.00	40.77
MOTA	2546	CD CA	PRO	371	-4.325	12.420	27.362	1.00	34.01
MOTA	2547	CB	PRO	371	-5.076	11.950	28.619	1.00	40.77
MOTA	2548 2549	CG	PRO	371	-4.226	10.810	29.103	1.00	40.77
MOTA	2550	C	PRO	371	-3.266	13.483	27.699	1.00	34.01
MOTA MOTA	2550 2551	0	PRO	371	-2.400	13.277	28.559	1.00	40.77
ATOM	2552	N	PRO	372	-3.331	14.638	27.011	1.00	14.63
MOTA	2553	CD	PRO	372	-4.378	14.947	26.018	1.00	28.09
MOTA	2554	CA	PRO	372	-2.420	15.770	27.183	1.00	14.63
ATOM	2555	СВ	PRO	372	-2.940	16.769	26.143	1.00	28.09
MOTA	2556	CG	PRO	372	-4.418	16.447	26.055	1.00	28.09
ATOM	2557	C	PRO	372	-2.499	16.334	28.598	1.00	14.63
ATOM	2558	Ō	PRO	372	-3.589	16.532	29.141	1.00	28.09
ATOM	2559	N	PRO	373	-1.335	16.504	29.245	1.00	51.40
MOTA	2560	CD	PRO	373	-0.041	16.052	28.704	1.00	51.87
ATOM	2561	CA	PRO	373	-1.181	17.035	30.609	1.00	51.40
MOTA	2562	CB	PRO	373	0.241	16.601	30.982	1.00	51.87
MOTA	2563	CG	PRO	373	0.963	16.653	29.668	1.00	51.87
MOTA	2564	C	PRO	373	-1.353	18.567	30.635	1.00 1.00	51.40 51.87
MOTA	2565	0	PRO	373	-0.819	19.271	29.765	1.00	42.06
MOTA	2566	N	ALA	374	-2.120	19.071	31.613 31.726	1.00	42.06
MOTA	2567	CA	ALA	374	-2.381	20.507 20.734	32.250	1.00	31.44
ATOM	2568	CB	ALA	374	-3.811 -1.350	21.373	32.499	1.00	42.06
ATOM	2569	C	ALA	374	-1.519	22.592	32.621	1.00	31.44
ATOM	2570	0	ALA ALA	374 375	-0.290	20.751	33.010	1.00	38.52
MOTA	2571	N CA	ALA	375	0.761	21.480	33.735	1.00	38.52
MOTA	2572	CB	ALA	375 375	1.602	22.327	32.752	1.00	29.54
MOTA	2573 2574	C	ALA	375	0.182	22.364	34.848	1.00	38.52
MOTA ATOM	2575	0	ALA	375	0.312	23.594	34.798	1.00	29.54
ATOM	2576	N	TYR	376	-0.385	21.710	35.874	1.00	47.67
ATOM	2577	CA		376	-1.024	22.369	37.024	1.00	47.67
ATOM	2578	CB		376	-0.030	23.174	37.857	1.00	78.81
ATOM	2579	CG		376	-0.681	23.843	39.065	1.00	78.81
ATOM	2580		1 TYR	376	-0.993	23.100	40.207	1.00	78.81
MOTA	2581		1 TYR	376	-1.555		41.345	1.00	78.81
ATOM	2582	CD	2 TYR	376	-0.954	25.218	39.085	1.00	78.81
MOTA	2583	CE	2 TYR	376	-1.520		40.228		78.81
MOTA	2584	CZ	TYR	376	-1.813		41.350		78.81
MOTA	2585	OH		376	-2.336		42.493		78.81
MOTA	2586		TYR	376	-2.129	_	36.564		47.67
MOTA	2587		TYR	376	-3.319		36.729		78.81 45.97
MOTA	2588		ALA	377	-1.714		36.029 35.526		45.97
MOTA	2589			377	-2.621				46.05
MOTA	2590			377	-2.819				45.97
MOTA	2591		ALA	377	-1.996				46.05
MOTA	2592	0	ALA	377	-2.274	25.555			



## FIG. 3SS

ATOM	2593	N	ALA	378	-1.112	27.019	34.430	1.00	45.78
MOTA	2594	CA	ALA	378	-0.422	27.673	33.312	1.00	45.78
MOTA	2595	CB	ALA	378	-1.391	28.607	32.545	1.00	26.15
ATOM	2596	C	ALA	378	0.814	28.450	33.785	1.00	45.78
MOTA	2597	0	ALA	378	1.016	29.599	33.400	1.00	26.15
ATOM	2598	N	ALA	379	1.645	27.807	34.607	1.00	29.23
ATOM	2599	CA	ALA	379	2.866	28.434	35.106	1.00	29.23
MOTA	2600	СВ	ALA	379	3.634	27.463	36.003	1.00	29.46
ATOM	2601	C	ALA	379	3.730	28.822	33.902	1.00	29.23
ATOM	2602	ō	ALA	379	4.216	27.940	33.183	1.00	29.46
ATOM	2603	N	LEU	380	3.862	30.128	33.644	1.00	45.66
ATOM	2604	CA	LEU	380	4.681	30.608	32.522	1.00	45.66
ATOM	2605	CB	LEU	380	4.506	32.117	32.319	1.00	31.66
ATOM	2606	CG	LEU	380	3.081	32.622	32.111	1.00	31.66
ATOM	2607		LEU	380	3.140	33.905	31.285	1.00	31.66
ATOM	2608		LEU	380	2.240	31.568	31.385	1.00	31.66
	2609	C	LEU	380	6.167	30.299	32.691	1.00	45.66
ATOM	2610	0	LEU	380	6.924	31.141	33.173	1.00	31.66
MOTA			ASP	381	6.586	29.114	32.248	1.00	30.99
MOTA	2611	N		381	7.983	28.706	32.378	1.00	30.99
ATOM	2612	CA	ASP		8.162	27.266	31.901	1.00	18.50
MOTA	2613	CB	ASP	381	7.219	26.300	32.596	1.00	18.50
MOTA	2614	CG	ASP	381		25.858	31.935	1.00	18.50
MOTA	2615		ASP	381	6.254		33.785	1.00	18.50
MOTA	2616		ASP	381	7.442	25.975	31.678	1.00	30.99
MOTA	2617	C	ASP	381	8.982	29.639		1.00	18.50
MOTA	2618	0	ASP	381	10.175	29.642	32.019	1.00	60.09
MOTA	2619	N	ALA	382	8.505	30.385	30.676		60.09
MOTA	2620	CA	ALA	382	9.324	31.366	29.951	1.00	
MOTA	2621	CB	ALA	382	8.879	31.475	28.520	1.00	18.75 60.09
MOTA	2622	С	ALA	382	9.055	32.684	30.706	1.00	
MOTA	2623	0	ALA	382	8.280	33.536	30.250	1.00	18.75 31.28
MOTA	2624	N	ARG	383	9.678	32.803	31.883	1.00	
MOTA	2625	CA	ARG	383	9.516	33.940	32.794	1.00	31.28
MOTA	2626	CB	ARG	383	8.867	33.415	34.072	1.00	38.51
MOTA	2627	CG	ARG	383	9.491	32.070	34.526	1.00	38.51
MOTA	2628	CD	ARG	383	8.900	31.514	35.807	1.00	38.51
MOTA	2629	NE	ARG	383	7.524	31.050	35.649	1.00	38.51
ATOM	2630	$\mathbf{cz}$	ARG	383	6.556	31.266	36.536	1.00	38.51
MOTA	2631		ARG	383	6.808	31.946	37.653	1.00	38.51
ATOM	2632	NH2	ARG	383	5.334	30.791	36.321	1.00	38.51
MOTA	2633	C	ARG	383	10.873	34.547	33.143	1.00	31.28
MOTA	2634	0	ARG	383	11.902	33.911	32.932	1.00	38.51
ATOM	2635	N	ALA	384	10.885	35.765	33.687	1.00	38.58
MOTA	2636	CA	ALA	384	12.148	36.409	34.067	1.00	38.58
ATOM	2637	CB	ALA	384	12.397	37.634	33.209	1.00	22.57
ATOM	2638	C	ALA	384	12.268	36.762	35.555	1.00	38.58
MOTA	2639	0	ALA	384	11.458	37.519	36.107	1.00	22.57
MOTA	2640	N	HIS	385	13.297	36.211	36.195	1.00	13.25
ATOM	2641	CA	HIS	385	13.545	36.434	37.618	1.00	13.25
ATOM	2642	CB	HIS	385	13.005	35.283	38.447	1.00	5.73
MOTA	2643	CG	HIS	385	11.537	35.076	38.326	1.00	5.73
ATOM	2644		HIS	385	10.803	34.416	37.402	1.00	5.73
ATOM	2645		. HIS	385	10.651	35.516	39.281	1.00	5.73
ATOM	2646		HIS	385	9.430	35.126	38.958	1.00	5.73
ATOM	2647		HIS	385	9.496	34.456	37.820	1.00	5.73
ATOM	2648	С	HIS	385	15.024	36.533	37.906	1.00	13.25
ATOM	2649	ō	HIS	385	15.859	36.234	37.065	1.00	5.73
ATOM	2650	N	THR	386	15.351	36.946	39.114	1.00	13.73
ATOM	2651	CA	THR		16.744	37.043	39.494		13.73



## FIG. 3TT

MOTA	2652	CB	THR	386	17.000	38.204	40.462	1.00	34.39
MOTA	2653	OG1	THR	386	15.920	38.298	41.406	1.00	34.39
MOTA	2654	CG2	THR	386	17.157	39.506	39.699	1.00	34.39
MOTA	2655	С	THR	386	17.138	35.762	40.185	1.00	13.73
MOTA	2656	0	THR	386	16.287	34.920	40.469	1.00	34.39
ATOM	2657	N	ILE	387	18.433	35.641	40.469	1.00	7.70
MOTA	2658	CA	ILE	387	19.008	34.499	41.162	1.00	7.70
MOTA	2659	CB	ILE	387	20.492	34.743	41.442	1.00	16.33
ATOM	2660	CG2	ILE	387	21.076	33.621	42.300	1.00	16.33
MOTA	2661	CG1	ILE	387	21.255	34.893	40.126	1.00	16.33
MOTA	2662	CD1	$_{ m ILE}$	387	22.736	35.136	40.334	1.00	16.33
MOTA	2663	C	ITĖ	387	18.286	34.300	42.491	1.00	7.70
MOTA	2664	0	ILE	387	17.898	33.188	42.815	1.00	16.33
MOTA	2665	N	ALA	388	18.098	35.379	43.247	1.00	2.00
MOTA	2666	CA	ALA	388	17.404	35.299	44.521	1.00	2.00
MOTA	2667	CB	ALA	388	17.384	36.658	45.183	1.00	28.05
MOTA	2668	C	ALA	388	15.984	34.762	44.363	1.00	2.00
MOTA	2669	0	ALA	388	15.559	33.901	45.128	1.00	28.05
MOTA	2670	N	GLU	389	15.264	35.246	43.353	1.00	18.37
MOTA	2671	CA	GLU	389	13.880	34.818	43.095	1.00	18.37
ATOM	2672	CB	GLU	389	13.183	35.797	42.161	1.00	30.68
MOTA	2673	CG	GLU	389	13.070	37.191	42.725	1.00	30.68
MOTA	2674	CD	GLU	389	12.680	38.226	41.684	1.00	30.68
MOTA	2675	OE1	GLU	389	12.475		40.503	1.00	30.68
MOTA	2676	OE2	GLU	389	12.583	39.408	42.051	1.00	30.68
MOTA	2677	C	GLU	389	13.800	33.431	42.483	1.00	18.37
MOTA	2678	0	GLU	389	12.827	32.704	42.706	1.00	30.68
MOTA	2679	N,	TRP	390	14.803	33.086	41.684	1.00	13.76
MOTA	2680	CA	TRP	390	14.858	31.786	41.044	1.00	13.76
MOTA	2681	CB	TRP	390	15.978	31.743	40.006	1.00	7.41
MOTA	2682	CG	TRP	390	15.576	32.219	38.639	1.00	7.41
MOTA	2683		TRP	390	14.552	31.663	37.790	1.00	7.41
MOTA	2684	CE2		390	14.564	32.401	36.591	1.00	7.41
MOTA	2685	CE3		390	13.619	30.632	37.935	1.00	7.41
ATOM	2686	CD1		390	16.149	33.229	37.932	1.00	7.41
ATOM	2687	NE1		390	15.554	33.341	36.701	1.00	7.41
ATOM	2688	CZ2		390	13.692	32.121	35.530	1.00	7.41
ATOM	2689	CZ3		390	12.750	30.358	36.883	1.00	7.41 7.41
ATOM	2690	CH2		390	12.789	31.104	35.700	1.00 1.00	13.76
MOTA	2691	C	TRP	390	15.116	30.733	42.110	1.00	7.41
ATOM	2692	0	TRP	390	14.447	29.707	42.144	1.00	3.15
ATOM	2693	N	LYS	391	16.074	31.011	42.987	1.00	3.15
ATOM	2694	CA	LYS	391	16.415	30.116	44.076 44.945	1.00	17.74
ATOM	2695	CB	LYS	391	17.491	30.768 30.047	44.345	1.00	17.74
ATOM	2696	CG	LYS	391	17.794	30.592	46.886	1.00	17.74
ATOM	2697	CD	LYS	391	19.069 19.494	29.775	48.113	1.00	17.74
ATOM	2698	CE	LYS	391	20.841	30.179	48.640	1.00	17.74
MOTA	2699	NZ	LYS	391		29.861	44.881	1.00	3.15
ATOM	2700	C	LYS	391	15.140 14.837	28.719	45.242	1.00	17.74
ATOM	2701	0	LYS	391 392	14.372	30.920	45.119	1.00	2.00
ATOM ATOM	2702	N CA	GLU GLU	392 392	13.126	30.920	45.859	1.00	2.00
	2703	CB	GLU	392 392	12.483	32.190	45.996	1.00	47.37
ATOM	2704		GLU	392 392	11.075	32.190	46.601	1.00	47.37
ATOM	2705	CG CD	GLU	392 392	11.075	32.162	48.104	1.00	47.37
ATOM ATOM	2706 2707		GLU	392	11.463	33.502	48.526	1.00	47.37
ATOM	2707	OE1		392 392	10.726	33.502	48.860	1.00	47.37
ATOM	2708	C C	GTO	392	12.151	29.896	45.141	1.00	2.00
ATOM	2709 2710	0	GLU	392	11.522	29.027	45.757	1.00	47.37
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FIG. 3UU

ATOM	2711	N	LEU	393	12.018	30.118	43.835	1.00	3.75
MOTA	2712	CA	LEU	393	11.114	29.356	42.990	1.00	3.75
MOTA	2713	CB	LEU	393	11.083	29.958	41.594	1.00	2.00
ATOM	2714	CG	LEU	393	10.159	31.146	41.373	1.00	2.00
MOTA	2715		LEU	393	10.352	31.661	39.962	1.00	2.00
MOTA	2716	CD2	LEU	393	8.727	30.707	41.598	1.00	2.00
MOTA	2717	C ´	LEU	393	11.487	27.894	42.882	1.00	3.75
MOTA	2718	0	LEU	393	10.620	27.029	42.840	1.00	2.00
MOTA	2719	N	ILE	394	12.787	27.632	42.857	1.00	11.25
MOTA	2720	CA	ILE	394	13.343	26.291	42.734	1.00	11.25
MOTA	2721	CB	ILE	394	14.839	26.396	42.406	1.00	2.00
MOTA	2722	CG2	ILE	394	15.516	25.028	42.423	1.00	2.00
MOTA	2723	CG1	ILE	394	14.969	27.090	41.050	1.00	2.00
MOTA	2724	CD1	ILE	394	16.345	27.169	40.524	1.00	2.00
MOTA	2725	С	ILE	394	13.104	25.456	43.980	1.00	11.25
MOTA	2726	0	ILE	394	12.649	24.313	43.901	1.00	2.00
ATOM	2727	N	TYR	395	13.391	26.058	45.127	1.00	24.41
ATOM	2728	CA	TYR	395	13.194	25.437	46.422	1.00	24.41
MOTA	2729	CB	TYR	395	13.752	26.378	47.492	1.00	24.18
ATOM	2730	CG	TYR	395	13.750	25.851	48.903	1.00	24.18
MOTA	2731	CD1		395	14.749	24.997	49.355	1.00	24.18
ATOM	2732	CE1	TYR	395	14.784	24.574	50.685	1.00	24.18
ATOM	2733		TYR	395	12.787	26.267	49.810	1.00	24.18
ATOM	2734	CE2	TYR	395	12.816	25.854	51.138	1.00	24.18
ATOM	2735	CZ	TYR	395	13.811	25.013	51.570	1.00	24.18
ATOM	2736	ОН	TYR	395	13.823	24.643	52.892	1.00	24.18
MOTA	2737	C	TYR	395	11.696	25.153	46.638	1.00	24.41
ATOM	2738	0	TYR	395	11.329	24.060	47.040	1.00	24.18
ATOM	2739	N	LYS	396	10.824	26.100	46.312	1.00	7.12
MOTA	2740	CA	LYS	396	9.387	25.887	46.486	1.00	7.12
ATOM	2741	CB	LYS	396	8.596	27.142	46.099	1.00	14.43
ATOM	2742	CG	LYS	396	8.648	28.257	47.134	1.00	14.43
ATOM	2743	CD	LYS	396	7.966	29.513	46.634	1.00	14.43
ATOM	2744	CE	LYS	396	7.873	30.571	47.723	1.00	14.43
MOTA	2745	NZ	LYS	396	7.321	31.859	47.188	1.00	14.43
MOTA	2746	C	LYS	396	8.851	24.689	45.711	1.00	7.12
MOTA	2747	0	LYS	396	7.824	24.118	46.082	1.00	14.43
ATOM	2748	N	GLU	397	9.549	24.318	44.640	1.00	27.91
ATOM	2749	CA	GLU	397	9.146	23.197	43.790	1.00	27.91
ATOM ATOM	2750 2751	CB CG	GLU	397 397	9.576 9.153	23.428 22.327	42.330	1.00	25.61
ATOM	2752	CD	GLU	397 397	7.720	22.327	41.339 40.856	1.00	25.61 25.61
ATOM	2753		GLU	397	7.134	23.535	41.111	1.00	25.61
ATOM	2754		GLU	397	7.134	21.526		1.00	25.61
ATOM	2755	C	GLU	397	9.752	21.926	44.309	1.00	27.91
ATOM	2756	o	GLU	397	9.094	20.855	44.301	1.00	25.61
ATOM	2757	Ŋ	VAL	398	11.003	21.976	44.761	1.00	19.14
ATOM	2758	CA	VAL	398	11.701	20.813	45.296	1.00	19.14
ATOM	2759	CB	VAL	398	13.206	21.106	45.592	1.00	2.00
ATOM	2760		VAL	398	13.200	19.825	45.941	1.00	2.00
ATOM	2761		VAL	398	13.857	21.769	44.402	1.00	2.00
MOTA	2762	C	VAL	398	11.016	20.382	46.594	1.00	19.14
ATOM	2763	Ö	VAL	398	10.810	19.185	46.829	1.00	2.00
ATOM	2764	N	MET	399	10.642	21.366	47.420	1.00	22.42
ATOM	2765	CA	MET	399	9.969	21.114	48.693	1.00	22.42
ATOM	2766	CB	MET	399	10.111	22.305	49.635	1.00	20.89
ATOM	2767	CG	MET	399	10.947	21.968	50.854	1.00	20.89
ATOM	2768	SD	MET	399	12.603	21.419	50.367	1.00	20.89
ATOM	2769	CE	MET	399	13.360	21.155	52.002	1.00	20.89
							_		



ATOM	2770	С	MET	399	8.504	20.808	48.455	1.00	22.42
ATOM	2771	0	MET	399	7.891	20.052	49.210	1.00	20.89
ATOM	2772	N	ASN	400	7.948	21.403	47.406	1.00	28.60
ATOM	2773	CA	ASN	400	6.565	21.150	47.049	1.00	28.60
ATOM	2774	CB	ASN	400	6.481	19.736	46.459	1.00	81.18
ATOM	2775	CG	ASN	400	5.100	19.387	45.951	1.00	81.18
MOTA	2776	OD1	ASN	400	4.599	18.282	46.199	1.00	81.18
ATOM	2777	ND2	ASN	400	4.479	20.318	45.219	1.00	81.18
ATOM	2778	C	ASN	400	5.629	21.282	48.257	1.00	28.60
ATOM	2779	0	ASN	400	5.257	22.426	48.589	1.00	81.18
MOTA	2780	C5	3400	1001	22.736	4.627	31.172	1.00	20.00
MOTA	2781	C2	3400	1001	22.276	5.904	31.111	1.00	20.00
MOTA	2782	Nl	3400	1001	23.156	6.818	30.322	1.00	20.00
MOTA	2783	C4	3400	1001	24.235	6.108	29.848	1.00	20.00
MOTA	2784	S1	3400	1001	24.123	4.375	30.081	1.00	20.00
MOTA	2785	C15	3400	1001	27.483	6.454	27.874	1.00	20.00
MOTA	2786	NЗ	3400	1001	27.589	7.776	27.927	1.00	20.00
MOTA	2787	C17	3400	1001	26.749	8.622	28.538	1.00	20.00
MOTA	2788	C11	3400	1001	25.618	8.113	29.190	1.00	20.00
MOTA	2789	C13	3400	1001	25.444	6.726	29.175	1.00	20.00
MOTA	2790	C19	3400	1001	26.367	5.887	28.516	1.00	20.00
MOTA	2791	C1	3400	1001	20.021	10.016	32.442	1.00	20.00
MOTA	2792	C9	3400	1001	19.766	8.582	32.361	1.00	20.00
MOTA	2793	C3	3400	1001	18.521 <sup>.</sup>	8.129	32.868	1.00	20.00
MOTA	2794	C12	3400	1001	17.569	9.048	33.425	1.00	20.00
MOTA	2795	C20	3400	1001	17.887	10.433	33.471	1.00	20.00
ATOM	2796	C6	3400	1001	19.111	11.000	32.997	1.00	20.00
ATOM	2797	C7	3400	1001	20.961	6.391	31.694	1.00	20.00
MOTA	2798	03	3400	1001	20.137	5.549	32.029	1.00	20.00
MOTA	2799	N2	3400	1001	20.762	7.730	31.764	1.00	20.00
MOTA	2800	C8	3400	1001	19.395	12.627	33.166	1.00	20.00
MOTA	2801	F3	3400	1001	20.299	13.330	32.210	1.00	20.00
MOTA	2802	F2	3400	1001	20.027	12.609	34.486	1.00	20.00
MOTA	2803	F1	3400	1001	18.169	13.443	33.069	1.00	20.00
					END				

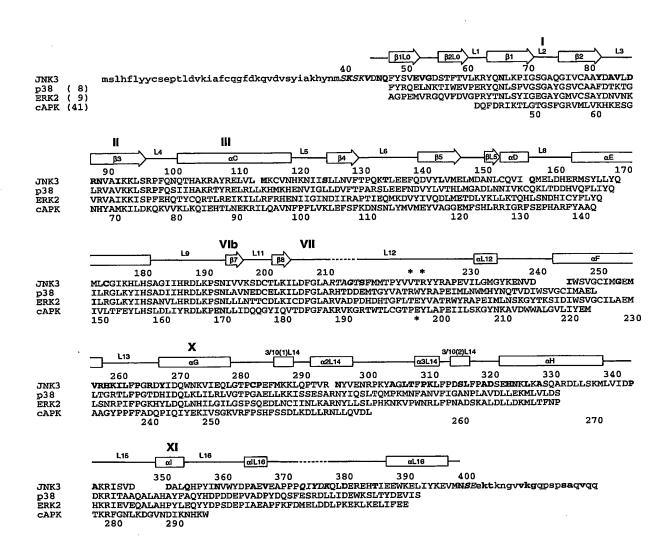
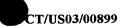


FIG.4



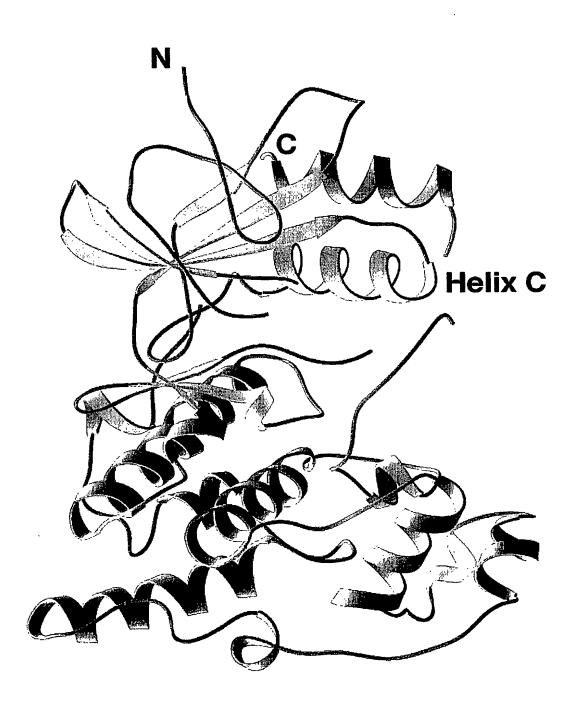


FIG. 5

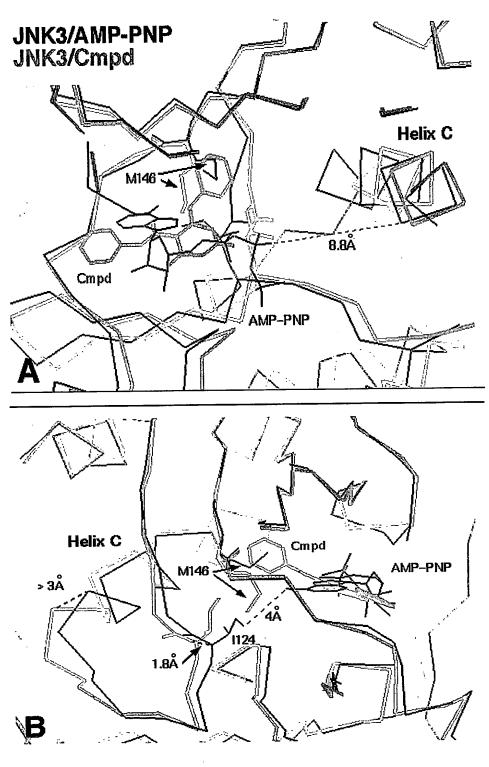


FIG.6

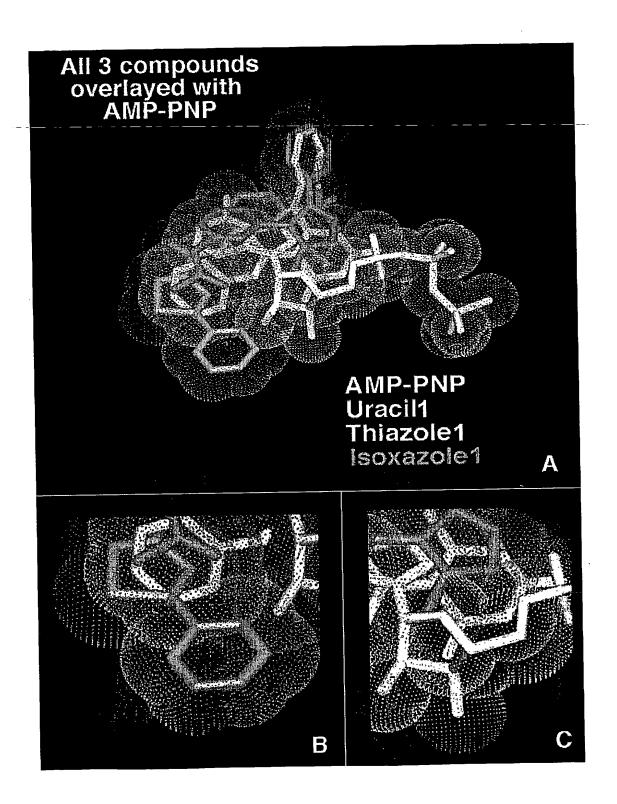
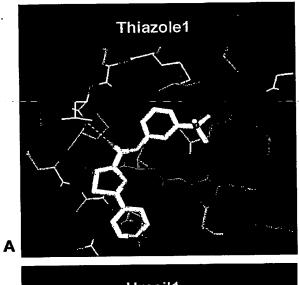
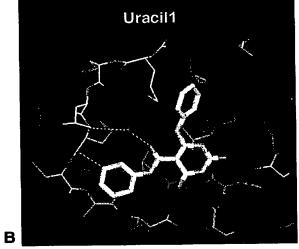


FIG.7





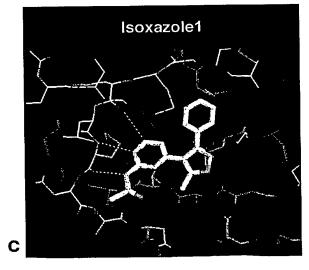


FIG.8

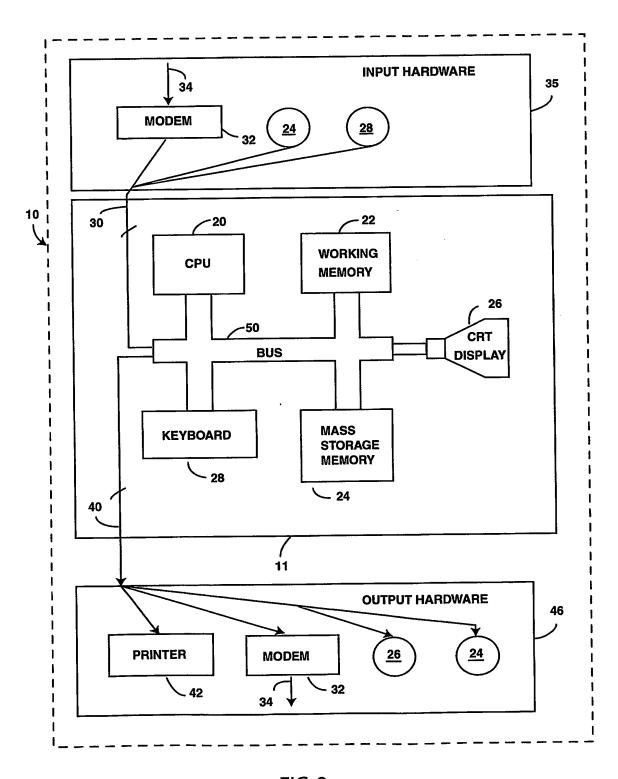
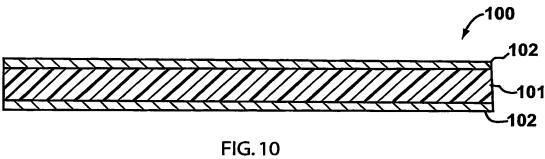


FIG.9





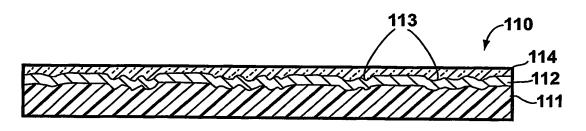


FIG. 11